

## Supplementary material

# Theoretical study for the Cl-initiated atmospheric oxidation of methyl isopropenyl ketone

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**Keywords:** Methyl isopropenyl ketone; Cl atom; Reaction mechanism; Kinetic parameters

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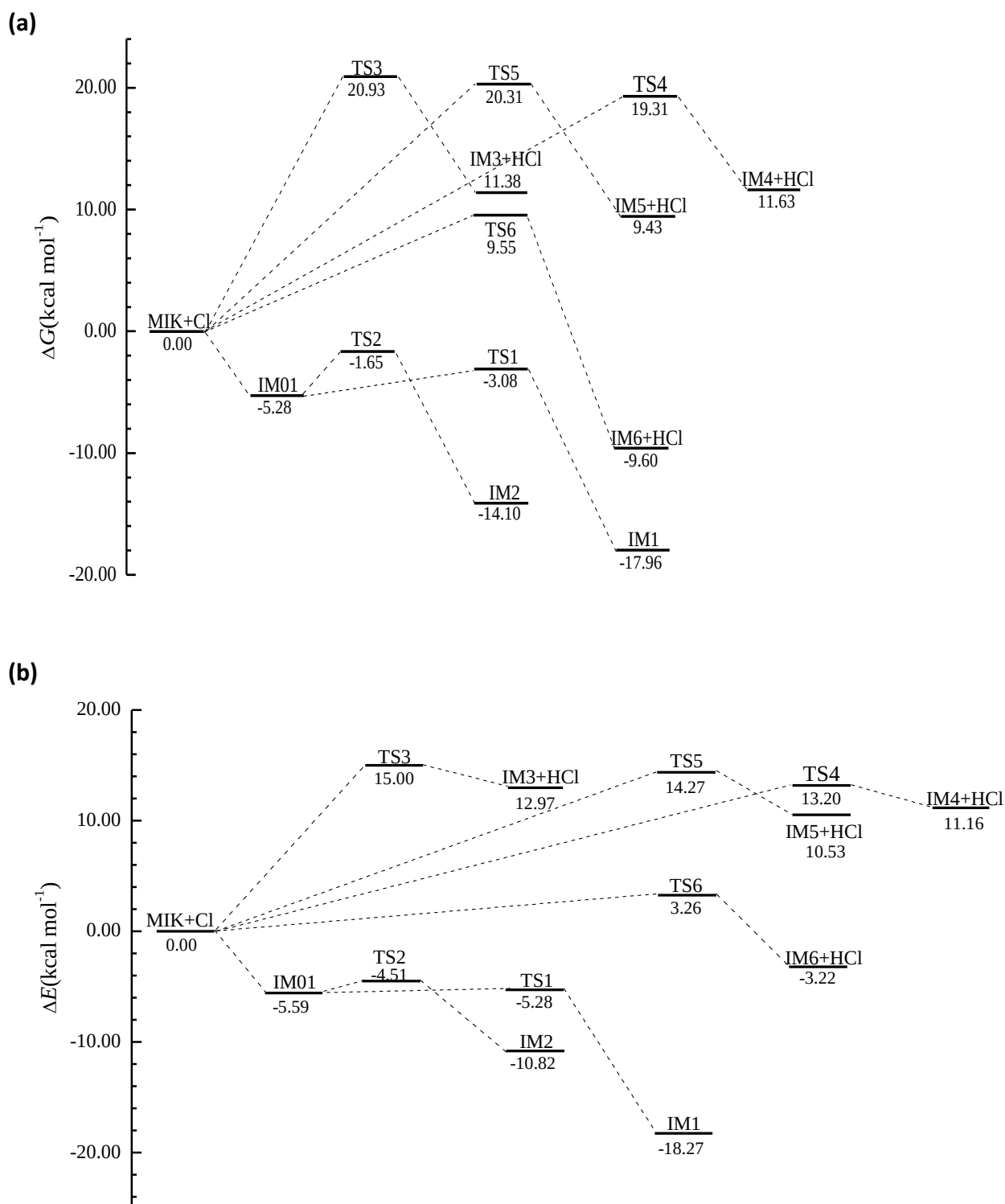
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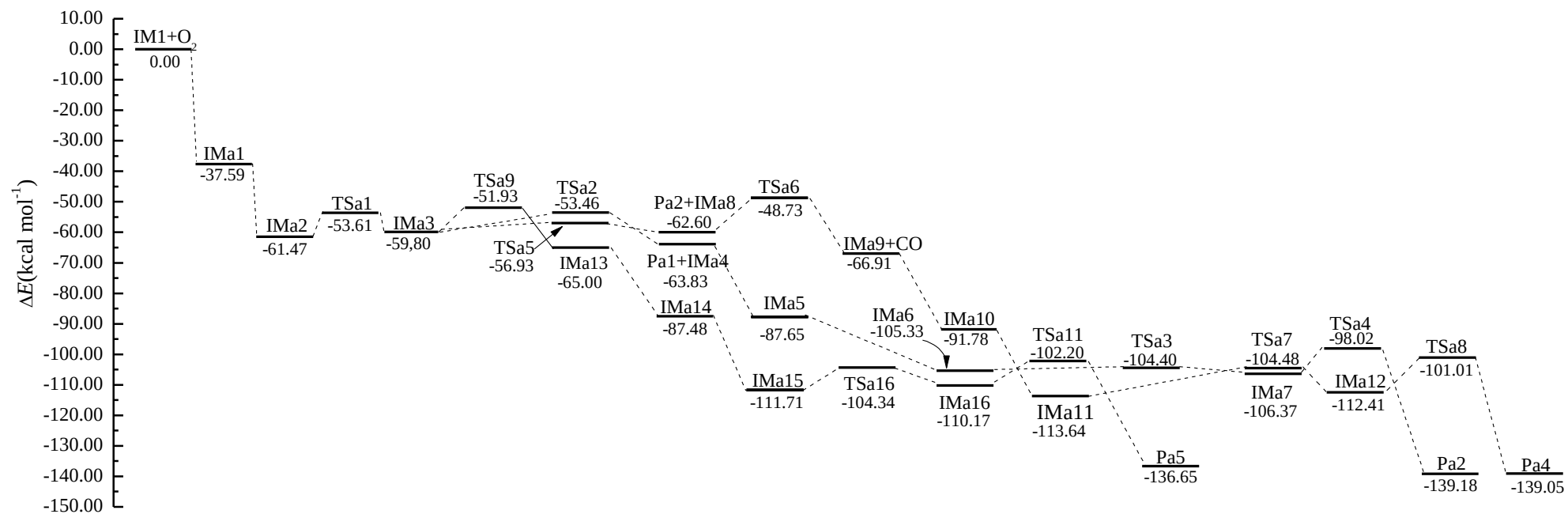
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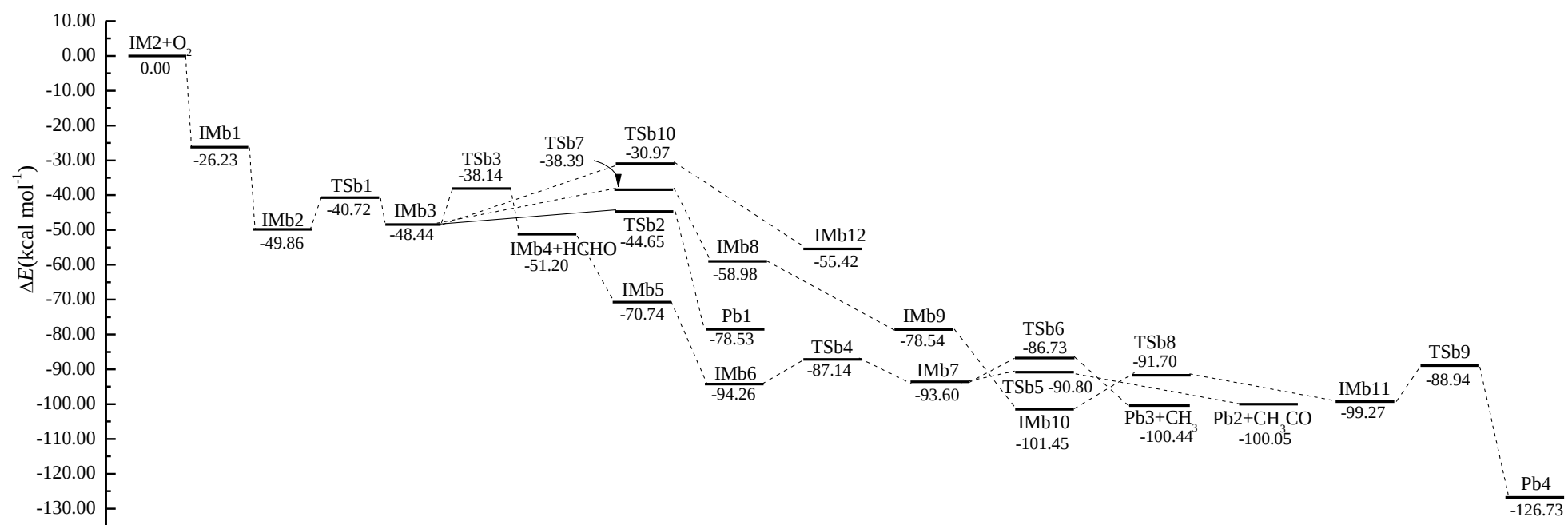


**Fig. S1. (a)** Profile of the free energy surface for the reaction pathways the reaction of MIK with Cl atoms at the CCSD(T)/6-311++G(d,p)//MP2/6-311G(d,p) level.

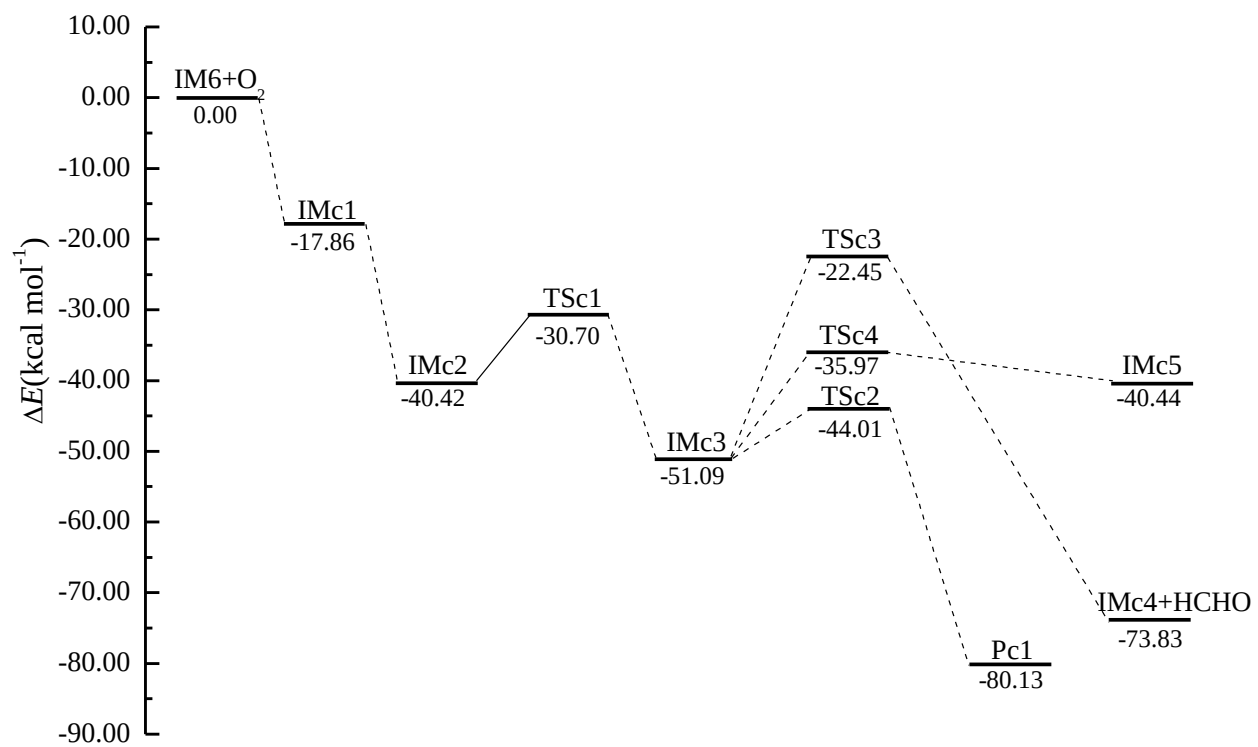
**(b)** Profile of the potential energy surface for the reaction of MIK with Cl atoms at the CCSD(T)/6-311++G(d,p)//MP2/6-311G(d,p) level.



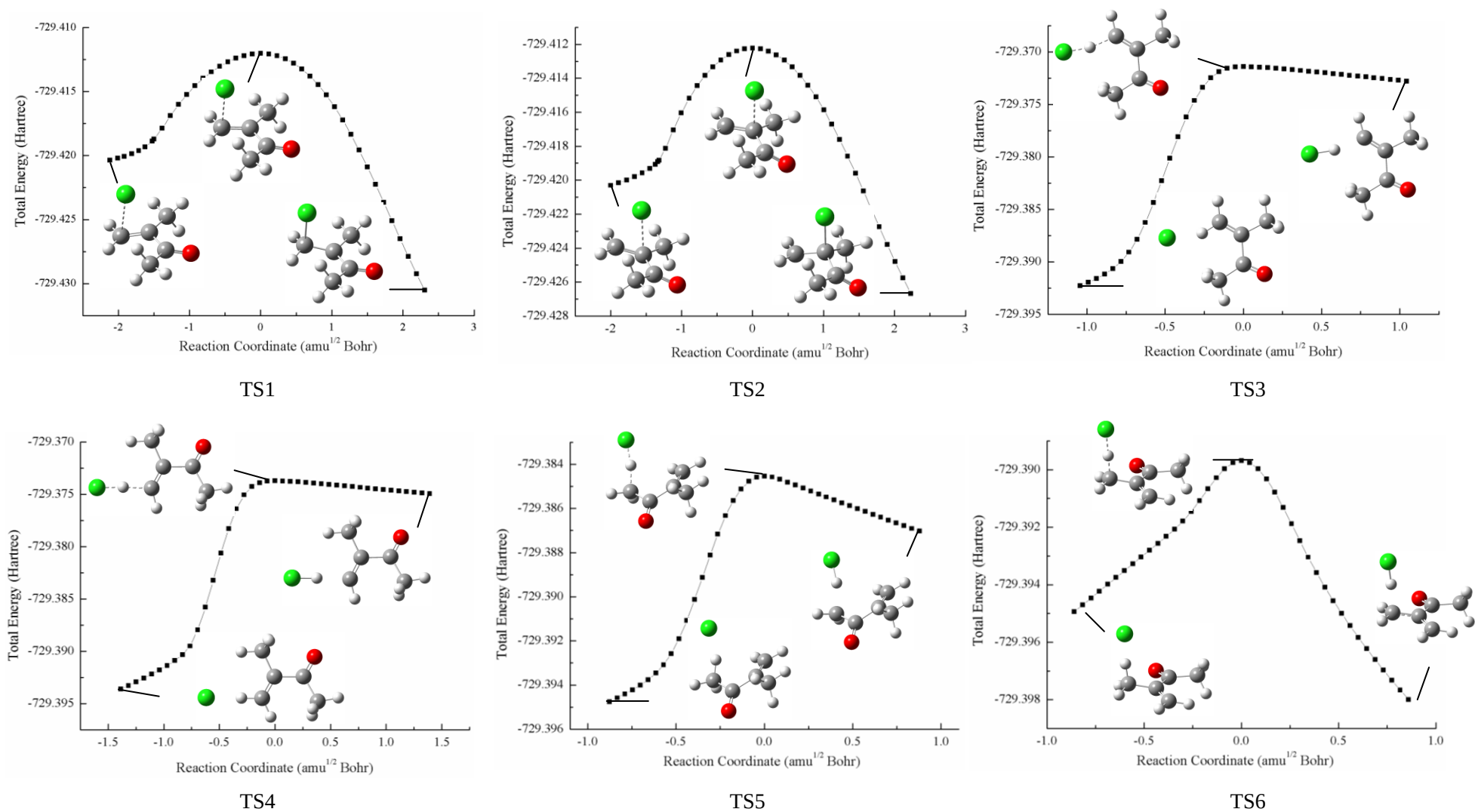
**Fig. S2.** Profile of the potential energy surface for the secondary reaction pathways of IM1.



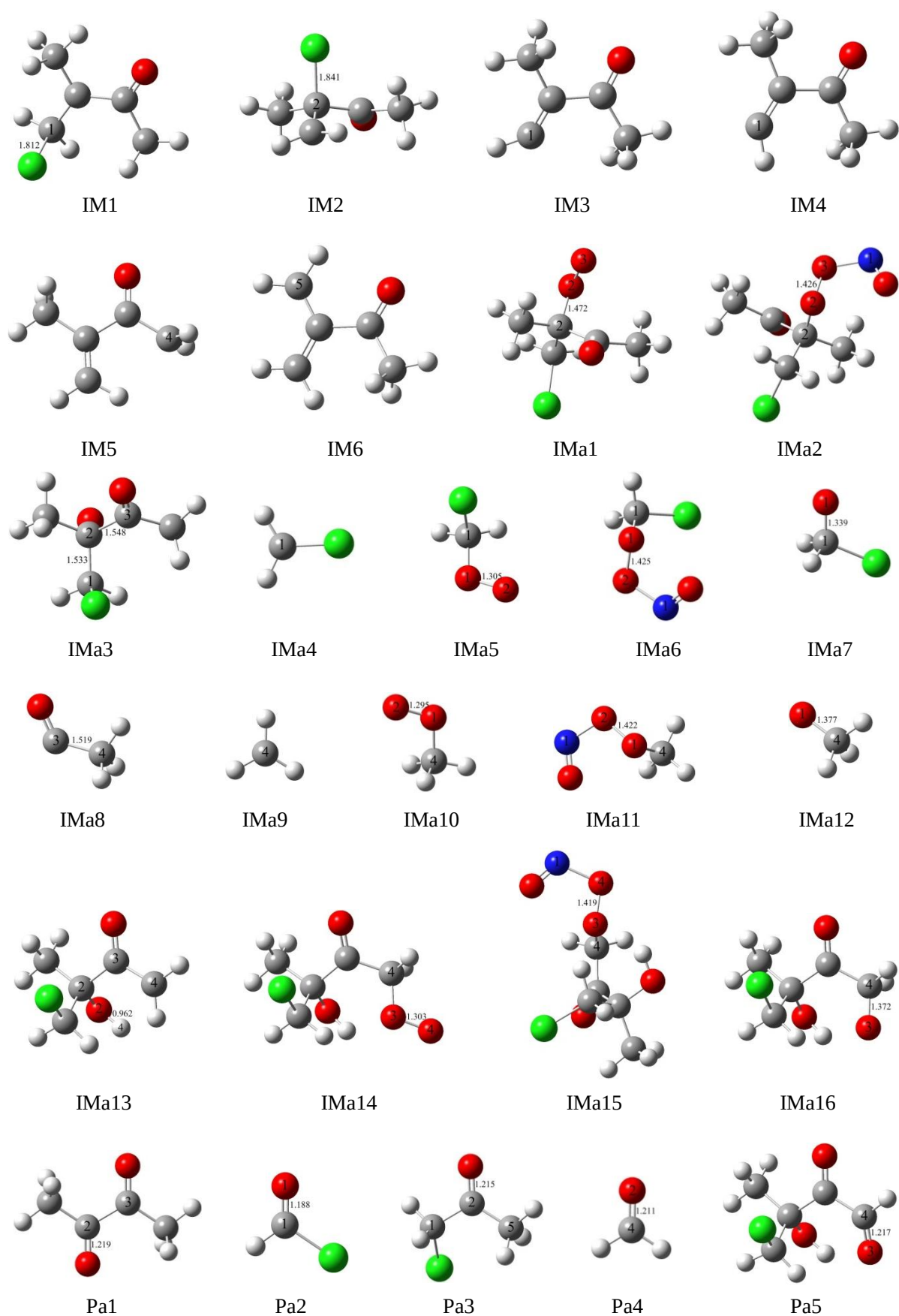
**Fig. S3.** Profile of the potential energy surface for the secondary reaction pathways of IM2.



**Fig. S4.** Profile of the potential energy surface for the secondary reaction pathways of IM6.

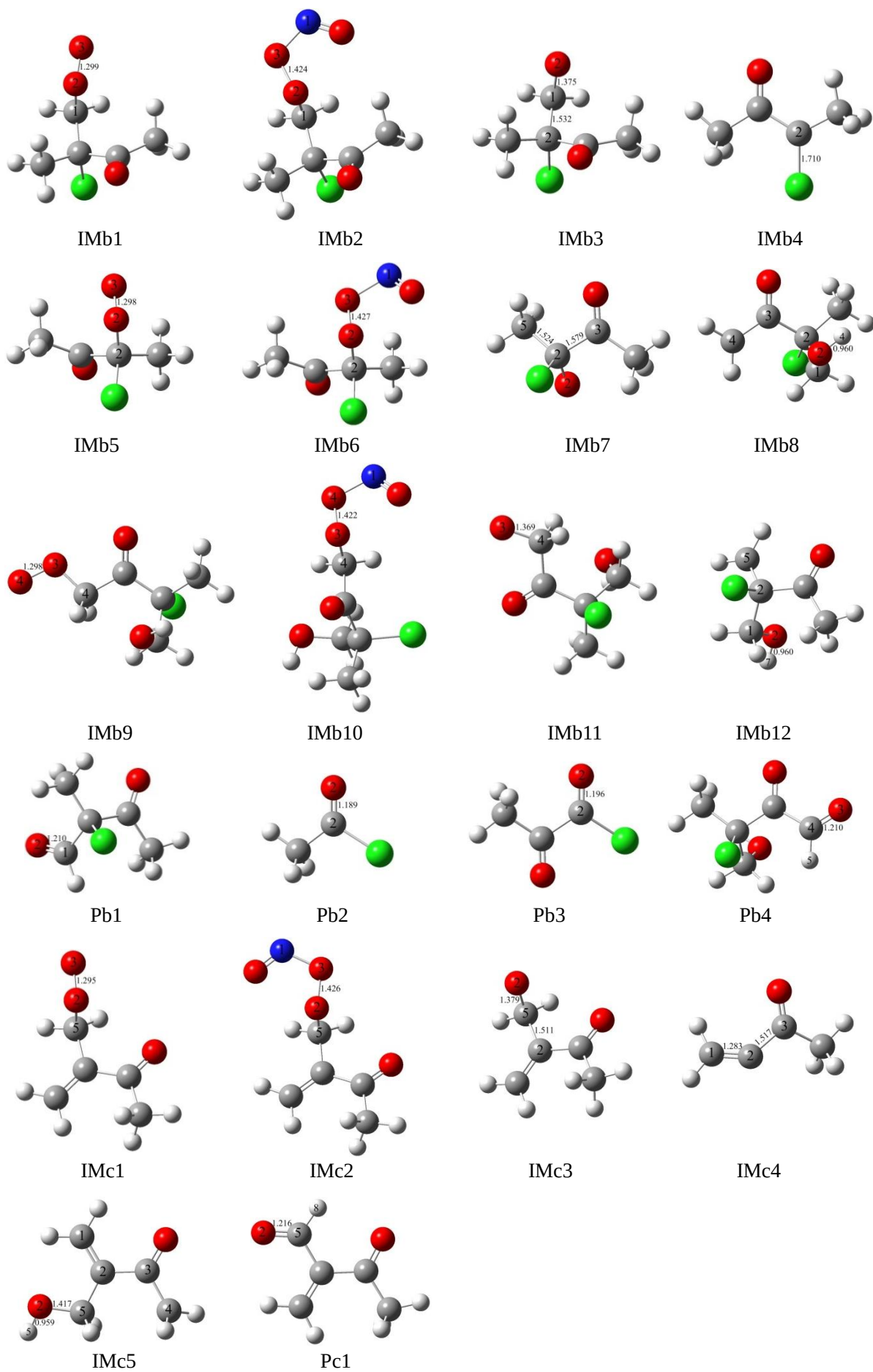


**Fig. S5.** The IRC trajectories of transition states for Cl addition pathways and H abstractions pathways

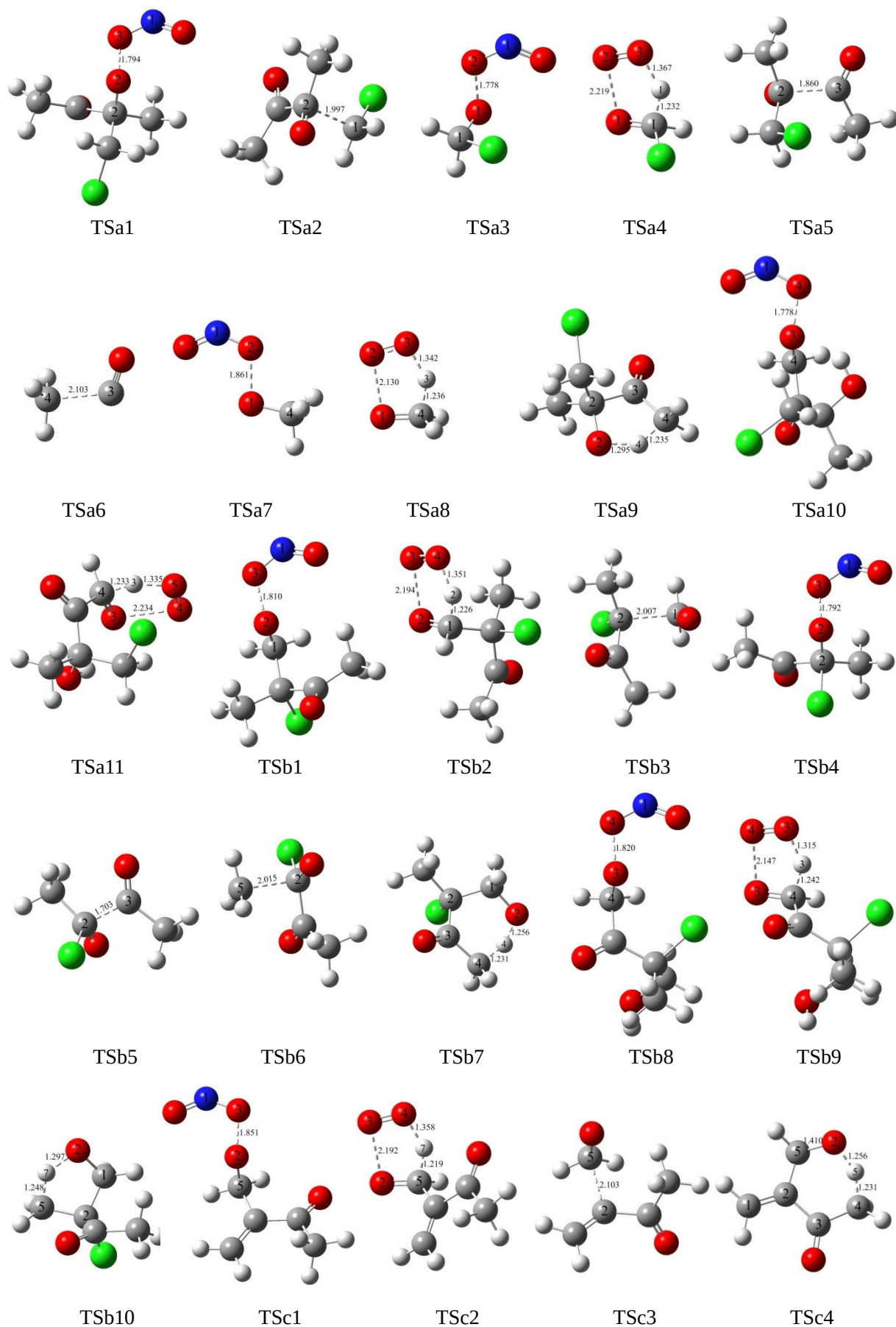


**Fig. S6.** MP2/6-311G(d,p) optimized geometries with the bond lengths (Å) for the intermediate states and products involved in the reaction of MIK with Cl atoms.





**Fig. S6. (continued)**



**Fig. S7** MP2/6-311G(d,p) optimized geometries with the bond lengths (Å) for the transition states involved in the reaction of MIK with Cl atoms.

**Table S1** The obtained zero point vibrational energy (ZPE), the Gibbs free energy(G), the Enthalpy(H), and the Entropy (S) of various species at the MP2/6-311G(d,p) level.

| Species | ZPE <sup>a</sup> | G <sup>a</sup> | H <sup>a</sup> | S <sup>b</sup> |
|---------|------------------|----------------|----------------|----------------|
| MIK     | -269.705787      | -269.736671    | -269.697691    | 82.039         |
| IM01    | -729.279216      | -729.313691    | -729.269618    | 92.760         |
| IM1     | -729.316444      | -729.351419    | -729.306852    | 93.799         |
| IM2     | -729.314323      | -729.348073    | -729.304630    | 91.433         |
| IM3     | -269.022763      | -269.054708    | -269.014640    | 84.330         |
| IM4     | -269.021627      | -269.053704    | -269.013542    | 84.528         |
| IM5     | -269.034986      | -269.066194    | -269.026975    | 82.544         |
| IM6     | -269.055107      | -269.086977    | -269.047360    | 83.381         |
| IMa1    | -879.366599      | -879.403376    | -879.355310    | 101.165        |
| IMa2    | -1009.029155     | -1009.068708   | -1009.015560   | 111.859        |
| IMa3    | -804.362540      | -804.397853    | -804.352263    | 95.952         |
| IMa4    | -498.737763      | -498.761902    | -498.733442    | 59.898         |
| IMa5    | -648.784632      | -648.813010    | -648.779413    | 70.710         |
| IMa6    | -778.449033      | -778.480232    | -778.441619    | 81.267         |
| IMa7    | -573.789126      | -573.815350    | -573.784785    | 64.330         |
| IMa8    | -152.755597      | -152.781390    | -152.750663    | 64.669         |
| IMa9    | -39.677120       | -39.696959     | -39.673038     | 50.348         |
| IMa10   | -189.725342      | -189.750987    | -189.720594    | 63.969         |
| IMa11   | -319.383896      | -319.412579    | -319.377300    | 74.250         |
| IMa12   | -114.722820      | -114.745749    | -114.718894    | 56.521         |
| IMa13   | -804.371190      | -804.406668    | -804.360624    | 96.909         |
| IMa14   | -954.423935      | -954.463096    | -954.411722    | 108.127        |
| IMa15   | -1084.087849     | -1084.129862   | -1084.073462   | 118.704        |
| IMa16   | -879.426265      | -879.462902    | -879.415306    | 100.175        |
| IMb1    | -879.366696      | -879.404311    | -879.355382    | 102.978        |
| IMb2    | -1009.028447     | -1009.067858   | -1009.015045   | 111.155        |
| IMb3    | -804.366578      | -804.401426    | -804.356385    | 94.797         |
| IMb4    | -690.152589      | -690.185291    | -690.144252    | 86.374         |
| IMb5    | -840.199224      | -840.233844    | -840.189304    | 93.742         |
| IMb6    | -969.862331      | -969.899617    | -969.850132    | 104.151        |
| IMb7    | -765.202851      | -765.236420    | -765.193657    | 90.001         |
| IMb8    | -804.374852      | -804.410038    | -804.364099    | 96.687         |
| IMb9    | -804.374900      | -804.409821    | -804.364517    | 95.350         |
| IMb10   | -954.421890      | -954.461283    | -954.409499    | 108.988        |
| IMb11   | -1084.082028     | -1084.123702   | -1084.067519   | 118.247        |

| Species | ZPE <sup>a</sup> | G <sup>a</sup> | H <sup>a</sup> | S <sup>b</sup> |
|---------|------------------|----------------|----------------|----------------|
| IMb12   | -879.421696      | -879.458091    | -879.410542    | 100.075        |
| IMc1    | -419.102612      | -419.138263    | -419.092724    | 95.845         |
| IMc2    | -548.762272      | -548.800647    | -548.750317    | 105.929        |
| IMc3    | -344.099104      | -344.132264    | -344.090330    | 88.258         |
| IMc4    | -229.848262      | -229.878181    | -229.841374    | 77.468         |
| IMc5    | -344.099641      | -344.133382    | -344.090207    | 90.868         |
| Pa1     | -305.627162      | -305.658482    | -305.619111    | 82.864         |
| Pa2     | -573.289234      | -573.314433    | -573.285067    | 61.808         |
| Pa3     | -651.620926      | -651.651179    | -651.614105    | 78.029         |
| Pa4     | -114.208199      | -114.229864    | -114.204389    | 53.617         |
| Pa5     | -878.915614      | -878.951113    | -878.904894    | 97.276         |
| Pb1     | -803.854280      | -803.889074    | -803.844136    | 94.581         |
| Pb2     | -612.469157      | -612.496832    | -612.463672    | 69.793         |
| Pb3     | -725.526118      | -725.557495    | -725.518723    | 81.603         |
| Pb4     | -878.906337      | -878.942732    | -878.895225    | 99.986         |
| Pc1     | -343.594464      | -343.626951    | -343.585903    | 86.392         |
| TS1     | -729.290673      | -729.325469    | -729.281241    | 93.086         |
| TS2     | -729.291231      | -729.324947    | -729.281998    | 90.394         |
| TS3     | -729.257101      | -729.294009    | -729.247305    | 98.297         |
| TS4     | -729.259624      | -729.296227    | -729.249593    | 98.151         |
| TS5     | -729.265467      | -729.300947    | -729.255765    | 95.093         |
| TS6     | -729.275178      | -729.311514    | -729.265462    | 96.926         |
| TSa1    | -1009.013063     | -1009.052731   | -1008.999814   | 111.372        |
| TSa2    | -804.336811      | -804.372847    | -804.326227    | 98.121         |
| TSa3    | -778.433272      | -778.464863    | -778.426110    | 81.563         |
| TSa4    | -723.799231      | -723.829172    | -723.793170    | 75.772         |
| TSa5    | -804.358971      | -804.394038    | -804.348744    | 95.329         |
| TSa6    | -152.728456      | -152.755577    | -152.722979    | 68.610         |
| TSa7    | -319.360193      | -319.391392    | -319.353401    | 79.961         |
| TSa8    | -264.725150      | -264.752221    | -264.720128    | 67.546         |
| TSa9    | -804.336386      | -804.371099    | -804.326687    | 93.473         |
| TSa10   | -1084.073004     | -1084.115252   | -1084.058888   | 118.629        |
| TSa11   | -1029.435974     | -1029.474750   | -1029.423270   | 108.348        |
| TSb1    | -1009.010491     | -1009.050582   | -1008.997261   | 112.223        |
| TSb2    | -954.376010      | -954.414282    | -954.363896    | 106.046        |
| TSb3    | -804.335304      | -804.370346    | -804.324969    | 95.503         |
| TSb4    | -969.846000      | -969.883966    | -969.833968    | 105.230        |
| TSb5    | -765.202901      | -765.236267    | -765.193913    | 89.141         |

| Species | ZPE <sup>a</sup> | G <sup>a</sup> | H <sup>a</sup> | S <sup>b</sup> |
|---------|------------------|----------------|----------------|----------------|
| TSb6    | -765.177161      | -765.211148    | -765.167775    | 91.287         |
| TSb7    | -804.329938      | -804.364087    | -804.320546    | 91.642         |
| TSb8    | -804.341792      | -804.375450    | -804.332514    | 90.366         |
| TSb9    | -1084.061723     | -1084.104570   | -1084.047265   | 120.608        |
| TSb10   | -1029.428601     | -1029.468962   | -1029.415496   | 112.529        |
| TSc1    | -548.740944      | -548.780514    | -548.728963    | 108.498        |
| TSc2    | -494.095815      | -494.132397    | -494.085341    | 99.036         |
| TSc3    | -344.039114      | -344.073804    | -344.029716    | 92.790         |
| TSc4    | -344.074372      | -344.106028    | -344.066586    | 83.013         |

*Note:* <sup>a</sup>ZPE, G, H are in Hartrees; <sup>b</sup>S is in cal mol<sup>-1</sup>.

**Table S2** The vibrational frequencies for the optimized stationary points

| Optimized stationary points | Vibrational frequencies (cm <sup>-1</sup> ) |           |            |
|-----------------------------|---------------------------------------------|-----------|------------|
| MIK                         | 64.897                                      | 158.4893  | 175.7784   |
|                             | 273.923                                     | 325.2462  | 381.5221   |
|                             | 454.6069                                    | 569.2206  | 577.7308   |
|                             | 720.9932                                    | 725.0852  | 913.6662   |
|                             | 941.9586                                    | 981.5892  | 1039.79    |
|                             | 1044.5132                                   | 1078.1301 | 1173.4842  |
|                             | 1355.1771                                   | 1405.3151 | 1425.165   |
|                             | 1457.3732                                   | 1491.9219 | 1494.5206  |
|                             | 1499.3719                                   | 1509.9031 | 1686.1376  |
|                             | 1737.691                                    | 3083.3423 | 3085.0307  |
|                             | 3166.021                                    | 3171.5748 | 3182.5155  |
|                             | 3185.8115                                   | 3205.2115 | 3282.7181  |
|                             | 3208.0122                                   | 3212.1065 | 3327.2705  |
| IM01                        | 62.9298                                     | 105.4902  | 161.6016   |
|                             | 169.0906                                    | 182.5012  | 253.5298   |
|                             | 276.6158                                    | 377.8296  | 446.5485   |
|                             | 522.4993                                    | 569.7914  | 685.5757   |
|                             | 714.5209                                    | 816.0242  | 943.1518   |
|                             | 982.3077                                    | 1036.0646 | 1039.4607  |
|                             | 1402.0258                                   | 1420.1541 | 1447.9575  |
|                             | 1482.1273                                   | 1491.7226 | 1447.9575  |
|                             | 1500.8823                                   | 1626.9909 | 1739.9804  |
|                             | 3085.0606                                   | 3087.2894 | 3167.8171  |
|                             | 3175.5646                                   | 3183.2393 | 3198.8726  |
|                             | 3209.5526                                   | 3301.2888 | 10371.3664 |
| IM1                         | 60.8825                                     | 82.8009   | 89.1871    |
|                             | 157.3917                                    | 186.2646  | 279.0126   |
|                             | 358.8005                                    | 372.1053  | 443.7006   |
|                             | 562.7984                                    | 602.9207  | 693.347    |
|                             | 724.4895                                    | 931.6152  | 959.4482   |
|                             | 985.85                                      | 994.3033  | 1058.8323  |
|                             | 1136.1161                                   | 1218.6516 | 1307.4036  |
|                             | 1339.0635                                   | 1369.3595 | 1403.415   |
|                             | 1416.9955                                   | 1482.0733 | 1492.7274  |
|                             | 1501.1019                                   | 1502.4437 | 1516.2192  |
|                             | 2128.2263                                   | 3053.378  | 3083.705   |
|                             | 3119.6287                                   | 3138.268  | 3171.1625  |
|                             | 3204.3824                                   | 3210.4275 | 3216.7843  |
| IM2                         | 72.0268                                     | 139.3921  | 185.809    |
|                             | 202.2387                                    | 263.6882  | 284.4786   |
|                             | 302.176                                     | 341.585   | 367.2895   |
|                             | 458.5885                                    | 508.6593  | 574.6359   |
|                             | 607.0676                                    | 664.0999  | 760.4926   |
|                             | 930.4078                                    | 977.8269  | 1009.9268  |
|                             | 1047.1327                                   | 1103.085  | 1167.339   |

|     |           |           |           |
|-----|-----------|-----------|-----------|
|     | 1273.9891 | 1304.5991 | 1401.2554 |
|     | 1427.449  | 1483.1749 | 1495.2169 |
|     | 1501.8912 | 1503.2103 | 1508.649  |
|     | 1775.3582 | 3087.4979 | 3090.6615 |
|     | 3178.4317 | 3182.3403 | 3205.9703 |
| IM3 | 44.4611   | 116.6152  | 195.482   |
|     | 256.0956  | 336.5347  | 350.0488  |
|     | 447.1948  | 572.3353  | 630.714   |
|     | 703.4258  | 866.7742  | 891.9246  |
|     | 957.782   | 1040.3649 | 1053.0645 |
|     | 1096.1599 | 1141.1775 | 1296.9608 |
|     | 1396.0428 | 1413.5454 | 1481.4729 |
|     | 1490.8161 | 1493.8437 | 1500.9316 |
|     | 1890.0098 | 2321.6311 | 3087.8144 |
|     | 3089.4582 | 3175.8438 | 3179.4182 |
|     | 3195.8041 | 3214.256  | 3296.0357 |
|     | 3119.6287 | 3138.268  | 3171.1625 |
|     | 3204.3824 | 3210.4275 | 3216.7843 |
| IM4 | 31.7704   | 137.514   | 194.6959  |
|     | 266.0685  | 353.9609  | 369.05    |
|     | 432.1451  | 572.0507  | 613.9141  |
|     | 716.761   | 855.3083  | 857.6199  |
|     | 958.6554  | 1043.8976 | 1058.4997 |
|     | 1101.7499 | 1147.3023 | 1281.4285 |
|     | 1393.331  | 1420.5298 | 1489.0264 |
|     | 1494.1093 | 1497.5524 | 1500.3071 |
|     | 1891.9271 | 2341.2094 | 3090.5385 |
|     | 3091.2514 | 3174.6303 | 3181.3576 |
|     | 3202.6034 | 3215.8274 | 3313.9508 |
| IM5 | 69.0985   | 196.2186  | 236.8965  |
|     | 252.0158  | 342.4509  | 350.0705  |
|     | 422.1614  | 557.4291  | 601.1596  |
|     | 630.6764  | 758.2417  | 819.1583  |
|     | 967.5386  | 1031.7823 | 1056.3641 |
|     | 1082.0504 | 1113.9902 | 1148.776  |
|     | 1369.743  | 1432.1605 | 1444.1748 |
|     | 1467.7871 | 1490.1476 | 1507.3621 |
|     | 2145.4093 | 3083.9426 | 3119.6905 |
|     | 3166.6706 | 3186.2672 | 3206.9272 |
| IM6 | 20.6085   | 181.0766  | 296.4192  |
|     | 350.399   | 396.6901  | 443.1673  |
|     | 559.1752  | 573.0687  | 583.5653  |
|     | 654.5784  | 720.2077  | 810.0029  |
|     | 823.4232  | 970.1601  | 986.9847  |
|     | 1060.5313 | 1066.4912 | 1186.4376 |
|     | 1288.7823 | 1387.5433 | 1414.701  |
|     | 1484.1317 | 1495.5193 | 1499.2341 |
|     | 1560.7966 | 2311.2767 | 3087.5746 |
|     | 3176.0668 | 3205.0516 | 3212.9169 |

|      |           |           |           |
|------|-----------|-----------|-----------|
|      | 3215.4557 | 3318.4563 | 3330.0297 |
| IMa1 | 76.1519   | 84.4163   | 97.3924   |
|      | 140.9322  | 158.932   | 206.424   |
|      | 248.2704  | 267.054   | 317.6589  |
|      | 354.605   | 364.1674  | 481.9167  |
|      | 495.9315  | 539.7395  | 664.3558  |
|      | 688.4433  | 823.4855  | 891.5383  |
|      | 927.8633  | 957.9247  | 1009.3546 |
|      | 1046.2472 | 1127.0473 | 1135.5596 |
|      | 1202.1811 | 1259.8187 | 1288.6218 |
|      | 1337.9463 | 1363.2365 | 1401.9172 |
|      | 1425.4169 | 1485.9852 | 1497.9447 |
|      | 1499.9201 | 1505.2041 | 1516.9316 |
|      | 1794.3207 | 3083.7929 | 3095.9072 |
|      | 3129.0169 | 3175.5259 | 3194.9875 |
|      | 3199.3067 | 3211.9994 | 3212.1447 |
| IMa2 | 50.5452   | 71.3923   | 75.7516   |
|      | 102.7601  | 123.8539  | 144.6921  |
|      | 178.9257  | 222.7008  | 266.194   |
|      | 278.3285  | 290.2958  | 307.8666  |
|      | 345.4802  | 373.3671  | 384.8377  |
|      | 489.5896  | 506.3837  | 542.4535  |
|      | 658.168   | 689.3213  | 777.7344  |
|      | 846.3531  | 898.6204  | 915.9955  |
|      | 944.3152  | 951.7795  | 1006.4908 |
|      | 1046.1433 | 1131.5783 | 1153.9816 |
|      | 1203.9277 | 1280.4073 | 1335.6666 |
|      | 1359.1378 | 1398.6344 | 1423.3285 |
|      | 1485.4753 | 1496.8145 | 1499.0338 |
|      | 1508.0362 | 1519.8484 | 1780.958  |
|      | 1794.8923 | 3082.2307 | 3095.0807 |
|      | 3130.8291 | 3174.6354 | 3194.5365 |
|      | 3202.5769 | 3203.5953 | 3212.7793 |
| IMa3 | 60.6859   | 94.6371   | 141.2345  |
|      | 171.1361  | 207.4399  | 245.2083  |
|      | 284.5663  | 328.6467  | 344.8408  |
|      | 401.4228  | 477.7134  | 541.5875  |
|      | 616.6805  | 682.6059  | 821.6207  |
|      | 887.3512  | 931.743   | 951.3086  |
|      | 995.853   | 1041.5517 | 1107.7141 |
|      | 1179.8734 | 1200.8085 | 1206.8234 |
|      | 1315.4467 | 1351.9335 | 1395.8053 |
|      | 1407.5618 | 1480.4134 | 1494.8482 |
|      | 1496.4752 | 1499.7458 | 1513.8239 |
|      | 1801.1228 | 3078.2564 | 3099.4924 |
|      | 3129.5917 | 3165.3929 | 3199.8801 |
|      | 3202.5112 | 3204.2329 | 3213.3958 |
| IMa4 | 277.592   | 876.6887  | 1047.8812 |
|      | 1472.7455 | 3235.8997 | 3390.6819 |



|       |           |           |           |
|-------|-----------|-----------|-----------|
| IMa5  | 115.6457  | 358.8194  | 544.1174  |
|       | 794.653   | 958.0711  | 1058.1306 |
|       | 1205.0275 | 1310.6899 | 1414.121  |
|       | 1480.1482 | 3162.7578 | 3254.2763 |
| IMa6  | 91.2538   | 113.0224  | 226.5061  |
|       | 288.0735  | 315.1711  | 404.7339  |
|       | 540.8872  | 747.9678  | 773.6127  |
|       | 903.1912  | 1021.878  | 1098.0764 |
|       | 1311.38   | 1406.14   | 1470.7205 |
|       | 1825.0002 | 3145.3438 | 3231.9946 |
| IMa7  | 413.0127  | 712.0976  | 740.6741  |
|       | 1120.0992 | 1122.1104 | 1368.6567 |
|       | 1384.9684 | 3056.2952 | 3118.1156 |
| IMa8  | 87.9538   | 469.1069  | 877.6268  |
|       | 960.0156  | 1062.1493 | 1369.6205 |
|       | 1481.5462 | 1483.0775 | 1947.2892 |
|       | 3080.3123 | 3189.8729 | 3195.5256 |
| IMa9  | 417.2157  | 1446.6548 | 1447.8107 |
|       | 3174.2198 | 3366.5589 | 3367.9018 |
| IMa10 | 142.8251  | 514.2204  | 973.8612  |
|       | 1165.7778 | 1216.7123 | 1286.5718 |
|       | 1486.6215 | 1499.432  | 1515.656  |
|       | 3107.0373 | 3218.1449 | 3232.9379 |
| IMa11 | 111.6524  | 201.9056  | 287.0616  |
|       | 353.2349  | 375.5357  | 512.1614  |
|       | 797.0591  | 931.6109  | 1056.958  |
|       | 1198.7391 | 1231.0806 | 1477.7825 |
|       | 1492.6498 | 1532.8307 | 1722.0523 |
|       | 3076.1732 | 3169.06   | 3196.497  |
| IMa12 | 820.5862  | 989.8756  | 1141.8051 |
|       | 1428.9075 | 1432.7829 | 1552.3641 |
|       | 3014.2521 | 3094.3781 | 3127.7691 |
| IMa13 | 48.9331   | 89.2003   | 172.1574  |
|       | 189.6719  | 230.05    | 255.5345  |
|       | 265.504   | 312.2971  | 361.646   |
|       | 368.7307  | 418.4739  | 485.0361  |
|       | 551.8401  | 581.5403  | 681.1935  |
|       | 796.8916  | 835.1572  | 898.7005  |
|       | 942.4288  | 986.0348  | 990.8747  |
|       | 1115.3861 | 1187.3462 | 1194.3619 |
|       | 1211.9889 | 1297.8543 | 1356.0451 |
|       | 1396.9493 | 1441.591  | 1478.7401 |
|       | 1495.4592 | 1503.7962 | 1513.6785 |
|       | 2131.8318 | 3098.0121 | 3116.3388 |
|       | 3186.8031 | 3196.4827 | 3205.4104 |
|       | 3213.9112 | 3334.0542 | 3867.9352 |
| IMa14 | 31.8801   | 53.6685   | 81.3013   |
|       | 102.8852  | 163.2907  | 182.073   |
|       | 226.2639  | 266.6618  | 282.5755  |

|       |           |           |           |
|-------|-----------|-----------|-----------|
|       | 345.1602  | 358.179   | 409.2512  |
|       | 427.2293  | 486.2934  | 517.5195  |
|       | 584.0758  | 651.2771  | 711.1334  |
|       | 836.9631  | 889.3611  | 970.0254  |
|       | 972.4629  | 1004.8651 | 1038.2057 |
|       | 1116.7572 | 1177.7875 | 1197.3964 |
|       | 1212.2212 | 1242.5717 | 1255.2821 |
|       | 1312.4926 | 1362.8638 | 1377.962  |
|       | 1404.7463 | 1443.724  | 1486.2512 |
|       | 1493.3005 | 1504.2775 | 1515.4931 |
|       | 1773.9846 | 3095.3084 | 3118.2496 |
|       | 3125.3556 | 3187.411  | 3199.2354 |
|       | 3203.5622 | 3215.4213 | 3848.8894 |
| IMa15 | 16.9969   | 46.5664   | 53.6559   |
|       | 97.8627   | 123.7159  | 138.8554  |
|       | 173.4055  | 223.5385  | 236.5613  |
|       | 270.8554  | 278.278   | 301.1925  |
|       | 341.8631  | 355.2021  | 370.9874  |
|       | 413.9519  | 430.7429  | 513.9894  |
|       | 574.4304  | 586.5145  | 657.5268  |
|       | 701.0456  | 806.8867  | 831.8515  |
|       | 887.9558  | 918.6259  | 969.1446  |
|       | 978.5395  | 1018.7101 | 1084.0622 |
|       | 1115.7374 | 1191.1736 | 1197.3044 |
|       | 1212.7809 | 1264.0544 | 1307.4969 |
|       | 1360.5748 | 1378.6883 | 1409.9761 |
|       | 1454.5943 | 1491.2104 | 1503.9737 |
|       | 1507.911  | 1515.3679 | 1771.142  |
|       | 1822.2771 | 3090.7525 | 3094.5599 |
|       | 3128.2518 | 3165.7698 | 3186.7329 |
|       | 3204.8027 | 3213.8454 | 3811.1888 |
| IMa16 | 40.3977   | 90.2462   | 108.2452  |
|       | 169.3073  | 213.7682  | 224.5379  |
|       | 269.7158  | 298.1582  | 353.8097  |
|       | 383.6338  | 423.0116  | 492.8082  |
|       | 541.3762  | 568.6521  | 635.6699  |
|       | 661.0484  | 830.9757  | 871.269   |
|       | 902.4491  | 963.9394  | 987.9133  |
|       | 1064.496  | 1108.1311 | 1170.8454 |
|       | 1176.8984 | 1194.0591 | 1208.0934 |
|       | 1284.0671 | 1314.4851 | 1359.1005 |
|       | 1406.1432 | 1412.7212 | 1452.5259 |
|       | 1493.598  | 1503.7277 | 1515.6079 |
|       | 1793.6865 | 2984.3541 | 3094.9369 |
|       | 3103.9662 | 3121.9302 | 3187.2568 |
|       | 3193.6507 | 3213.1043 | 3826.1828 |
| IMb1  | 25.8948   | 67.3309   | 125.295   |
|       | 151.0602  | 184.8658  | 198.7832  |
|       | 276.5774  | 285.7468  | 301.8045  |

|      |           |           |           |
|------|-----------|-----------|-----------|
|      | 359.4524  | 379.1504  | 428.7035  |
|      | 467.6892  | 558.8195  | 599.8383  |
|      | 705.6836  | 809.7546  | 949.3967  |
|      | 969.4001  | 998.0878  | 1028.4909 |
|      | 1051.617  | 1129.5526 | 1158.7625 |
|      | 1225.5218 | 1256.473  | 1274.3289 |
|      | 1329.9041 | 1402.26   | 1404.7577 |
|      | 1431.0375 | 1487.7227 | 1498.2293 |
|      | 1502.5841 | 1505.2654 | 1520.602  |
|      | 1779.0719 | 3085.1874 | 3092.0193 |
|      | 3121.3168 | 3175.4397 | 3184.98   |
|      | 3203.6999 | 3207.6581 | 3209.5312 |
| IMb2 | 40.0341   | 62.6054   | 78.7136   |
|      | 112.0066  | 152.0299  | 182.3821  |
|      | 193.3946  | 246.8016  | 268.1031  |
|      | 290.7881  | 299.7227  | 339.0877  |
|      | 344.6929  | 367.7397  | 394.5226  |
|      | 447.7112  | 471.3623  | 556.1207  |
|      | 596.2696  | 698.9308  | 798.3496  |
|      | 840.1117  | 927.6842  | 950.0266  |
|      | 986.1926  | 1011.995  | 1052.6529 |
|      | 1076.4171 | 1133.0623 | 1165.6579 |
|      | 1244.8185 | 1254.805  | 1332.6243 |
|      | 1401.0546 | 1410.6805 | 1433.0353 |
|      | 1492.8579 | 1497.927  | 1501.4954 |
|      | 1505.3211 | 1533.1181 | 1729.8938 |
|      | 1776.3143 | 3089.6907 | 3092.8626 |
|      | 3094.7794 | 3159.7942 | 3181.88   |
|      | 3189.5265 | 3207.3942 | 3208.3257 |
| IMb3 | 66.8823   | 114.7027  | 176.6613  |
|      | 196.7187  | 201.4291  | 280.5876  |
|      | 289.0844  | 314.2777  | 362.5558  |
|      | 403.8953  | 461.9148  | 531.0562  |
|      | 581.6637  | 614.143   | 695.6159  |
|      | 814.0742  | 944.9156  | 1003.0681 |
|      | 1034.6489 | 1059.5186 | 1083.3862 |
|      | 1121.8863 | 1191.8441 | 1247.8036 |
|      | 1320.6951 | 1378.9076 | 1400.9366 |
|      | 1411.6216 | 1430.3818 | 1492.0132 |
|      | 1500.133  | 1502.4614 | 1505.5137 |
|      | 1775.8862 | 3025.4707 | 3071.483  |
|      | 3084.5003 | 3087.309  | 3174.346  |
|      | 3178.6442 | 3205.8687 | 3208.0955 |
| IMb4 | 81.2813   | 94.831    | 178.1573  |
|      | 236.9627  | 244.6484  | 323.6016  |
|      | 443.2888  | 480.0981  | 576.3826  |
|      | 659.3693  | 885.8263  | 978.6147  |
|      | 1005.9149 | 1055.7082 | 1138.3302 |
|      | 1198.4883 | 1335.4001 | 1407.083  |

|      |           |           |           |
|------|-----------|-----------|-----------|
|      | 1410.1222 | 1481.5669 | 1491.3144 |
|      | 1492.4959 | 1496.7525 | 2095.2409 |
|      | 3066.2153 | 3093.6181 | 3136.7851 |
|      | 3180.1754 | 3204.9894 | 3222.3383 |
| IMb5 | 71.8889   | 124.1255  | 164.2641  |
|      | 193.436   | 215.076   | 271.1833  |
|      | 284.4299  | 320.2568  | 357.7688  |
|      | 434.2716  | 500.8309  | 557.2107  |
|      | 578.922   | 688.9411  | 825.1416  |
|      | 901.5086  | 1004.6215 | 1043.4019 |
|      | 1124.7825 | 1142.927  | 1173.9447 |
|      | 1259.4601 | 1287.4881 | 1407.725  |
|      | 1423.0234 | 1486.1312 | 1492.7667 |
|      | 1496.9928 | 1502.8988 | 1791.1968 |
|      | 3095.58   | 3103.8383 | 3186.6397 |
|      | 3205.2993 | 3213.3596 | 3217.9045 |
| IMb6 | 54.0271   | 88.246    | 95.0611   |
|      | 161.7076  | 168.2484  | 193.3089  |
|      | 220.4952  | 284.0185  | 295.5907  |
|      | 311.0713  | 328.9932  | 336.5809  |
|      | 377.6696  | 446.0509  | 513.8275  |
|      | 553.767   | 578.9367  | 689.9416  |
|      | 775.3578  | 826.3519  | 890.9925  |
|      | 930.1526  | 1006.9078 | 1042.5603 |
|      | 1133.3076 | 1150.4857 | 1198.7276 |
|      | 1294.5773 | 1405.495  | 1419.9951 |
|      | 1484.1158 | 1492.4746 | 1495.6358 |
|      | 1512.0118 | 1786.4089 | 1846.5302 |
|      | 3094.0694 | 3102.1362 | 3185.0291 |
|      | 3201.0664 | 3212.682  | 3215.8984 |
| IMb7 | 61.5763   | 147.5714  | 182.5953  |
|      | 227.083   | 248.9574  | 286.8252  |
|      | 305.1235  | 389.8494  | 423.0403  |
|      | 499.433   | 563.8018  | 629.9006  |
|      | 729.5433  | 921.8149  | 962.0845  |
|      | 1006.3754 | 1062.9567 | 1105.4411 |
|      | 1143.5647 | 1227.1792 | 1400.1648 |
|      | 1409.5792 | 1480.0971 | 1492.1831 |
|      | 1494.634  | 1498.9335 | 1820.6832 |
|      | 3086.6388 | 3102.3455 | 3177.8035 |
|      | 3205.9732 | 3215.6296 | 3220.7774 |
| IMb8 | 65.8633   | 140.4012  | 189.4324  |
|      | 195.2104  | 208.7616  | 219.7118  |
|      | 232.8247  | 285.441   | 301.7463  |
|      | 379.5978  | 392.7472  | 462.0719  |
|      | 535.0562  | 564.412   | 576.84    |
|      | 693.6533  | 816.0726  | 923.8208  |
|      | 990.6174  | 1001.2783 | 1057.6809 |
|      | 1105.0179 | 1166.9461 | 1213.3469 |

|       |           |           |           |
|-------|-----------|-----------|-----------|
|       | 1259.4287 | 1301.1335 | 1354.7728 |
|       | 1399.8206 | 1465.078  | 1478.475  |
|       | 1493.7599 | 1501.6151 | 1546.8036 |
|       | 1789.811  | 3063.3992 | 3088.5393 |
|       | 3121.5845 | 3180.7498 | 3207.9534 |
|       | 3218.52   | 3350.6837 | 3901.9847 |
| IMb9  | 71.3793   | 90.4024   | 190.9182  |
|       | 199.0366  | 268.4195  | 270.392   |
|       | 295.9805  | 318.458   | 340.0367  |
|       | 369.1633  | 413.5084  | 467.384   |
|       | 521.1218  | 598.5101  | 661.5968  |
|       | 776.7489  | 842.3041  | 939.9788  |
|       | 976.0444  | 1000.3548 | 1106.2915 |
|       | 1119.3516 | 1142.9684 | 1219.2503 |
|       | 1238.5564 | 1329.3395 | 1396.9894 |
|       | 1424.5031 | 1436.4936 | 1477.3857 |
|       | 1496.5915 | 1506.0814 | 1522.9872 |
|       | 2109.1669 | 3067.7413 | 3088.6174 |
|       | 3171.3885 | 3181.4133 | 3201.3382 |
|       | 3219.5016 | 3353.4219 | 3899.9143 |
| IMb10 | 24.8863   | 57.7052   | 89.3068   |
|       | 120.5538  | 161.7562  | 195.3223  |
|       | 205.7027  | 271.7337  | 282.6177  |
|       | 312.6057  | 331.7601  | 346.0723  |
|       | 401.3723  | 450.6464  | 488.0169  |
|       | 526.7641  | 612.5212  | 773.0746  |
|       | 854.2557  | 924.5371  | 973.105   |
|       | 998.4554  | 1033.7979 | 1100.0001 |
|       | 1110.1294 | 1115.5442 | 1180.4047 |
|       | 1246.4913 | 1264.7632 | 1280.7081 |
|       | 1316.5234 | 1397.3201 | 1417.448  |
|       | 1422.2072 | 1435.7311 | 1491.7923 |
|       | 1497.9526 | 1508.8221 | 1528.3621 |
|       | 1785.1976 | 3079.4738 | 3084.8346 |
|       | 3109.4742 | 3169.0736 | 3174.562  |
|       | 3181.6425 | 3204.2021 | 3902.0329 |
| IMb11 | 26.6923   | 37.8405   | 66.1147   |
|       | 99.4103   | 123.648   | 161.0497  |
|       | 197.1794  | 203.4021  | 261.8883  |
|       | 274.3655  | 276.8035  | 310.9967  |
|       | 315.6301  | 331.853   | 348.9522  |
|       | 363.8429  | 404.4294  | 455.2866  |
|       | 497.4099  | 536.5857  | 609.4321  |
|       | 759.199   | 815.3641  | 868.5815  |
|       | 928.8714  | 933.1761  | 974.5454  |
|       | 1021.8462 | 1056.9538 | 1100.5312 |
|       | 1113.6876 | 1139.7195 | 1185.3089 |
|       | 1247.9134 | 1288.0046 | 1316.1993 |
|       | 1398.2608 | 1418.4003 | 1422.2178 |

|       |           |           |           |
|-------|-----------|-----------|-----------|
|       | 1435.9682 | 1497.3601 | 1508.0864 |
|       | 1514.8403 | 1529.6952 | 1746.0234 |
|       | 1783.005  | 3076.5725 | 3077.9288 |
|       | 3084.2205 | 3138.5048 | 3170.3161 |
|       | 3173.6857 | 3204.1619 | 3902.1824 |
| IMb12 | 58.0992   | 98.2868   | 128.1687  |
|       | 188.6937  | 195.1206  | 232.0397  |
|       | 274.7436  | 302.0096  | 322.3596  |
|       | 344.4975  | 355.7582  | 403.2973  |
|       | 477.7709  | 496.6216  | 585.6457  |
|       | 723.3319  | 809.033   | 832.9784  |
|       | 927.8067  | 973.8651  | 1061.7975 |
|       | 1097.695  | 1105.3397 | 1117.1143 |
|       | 1173.5821 | 1184.4825 | 1244.884  |
|       | 1312.0228 | 1370.1072 | 1396.5122 |
|       | 1420.7202 | 1424.7315 | 1436.1557 |
|       | 1497.5671 | 1507.5355 | 1527.9776 |
|       | 1812.4001 | 3008.8138 | 3077.4023 |
|       | 3083.3029 | 3085.3161 | 3172.1462 |
|       | 3173.7785 | 3203.8346 | 3900.4638 |
| IMc1  | 43.5377   | 55.7963   | 87.4884   |
|       | 153.0638  | 172.1762  | 280.0218  |
|       | 374.1014  | 389.2393  | 407.4835  |
|       | 531.512   | 568.0962  | 640.2084  |
|       | 725.4037  | 746.0018  | 942.2601  |
|       | 965.1104  | 984.4569  | 1012.1256 |
|       | 1027.3765 | 1052.6489 | 1171.9627 |
|       | 1256.9432 | 1279.8872 | 1357.8866 |
|       | 1403.7457 | 1426.7059 | 1464.4708 |
|       | 1494.1649 | 1498.5027 | 1505.4534 |
|       | 1702.4943 | 1771.9746 | 3084.559  |
|       | 3125.2784 | 3170.5839 | 3187.8697 |
|       | 3207.7153 | 3208.4335 | 3285.9645 |
| IMc2  | 36.4453   | 39.3868   | 57.6307   |
|       | 106.298   | 140.3539  | 163.7675  |
|       | 254.4266  | 290.041   | 344.3894  |
|       | 377.3284  | 393.6162  | 418.2756  |
|       | 430.1165  | 525.8878  | 569.8173  |
|       | 639.6788  | 725.9787  | 740.6765  |
|       | 838.5124  | 927.4285  | 940.7311  |
|       | 974.1249  | 984.2412  | 1040.4848 |
|       | 1051.5329 | 1074.6982 | 1173.2413 |
|       | 1272.0971 | 1356.231  | 1404.7341 |
|       | 1425.1322 | 1463.0768 | 1494.0018 |
|       | 1498.7002 | 1524.3156 | 1685.1879 |
|       | 1705.1899 | 1749.3952 | 3084.3823 |
|       | 3092.754  | 3170.4854 | 3175.7219 |
|       | 3186.1928 | 3207.2834 | 3284.5956 |
| IMc3  | 62.1647   | 85.5464   | 154.2936  |

|      |           |           |           |
|------|-----------|-----------|-----------|
|      | 194.3659  | 276.2895  | 361.9185  |
|      | 417.8822  | 463.1167  | 555.6102  |
|      | 650.6629  | 714.5453  | 720.5785  |
|      | 849.5859  | 910.8964  | 952.8418  |
|      | 991.1192  | 1048.5843 | 1083.9211 |
|      | 1145.7946 | 1209.6672 | 1347.6473 |
|      | 1367.7394 | 1410.984  | 1422.862  |
|      | 1469.2331 | 1493.76   | 1498.9887 |
|      | 1674.6415 | 1995.8734 | 3028.7901 |
|      | 3083.7306 | 3084.2437 | 3169.8559 |
|      | 3188.0461 | 3206.0453 | 3280.7862 |
| IMc4 | 73.6907   | 140.7721  | 221.0845  |
|      | 363.4435  | 477.3859  | 595.1697  |
|      | 674.5712  | 746.6508  | 976.7191  |
|      | 1024.5044 | 1082.2329 | 1089.903  |
|      | 1221.4992 | 1396.6158 | 1424.7571 |
|      | 1478.1711 | 1488.7263 | 1924.7936 |
|      | 2393.6255 | 3082.1841 | 3145.0989 |
|      | 3169.8938 | 3214.8914 | 3256.8956 |
| IMc5 | 54.516    | 76.2895   | 191.8416  |
|      | 196.6136  | 216.1192  | 312.5218  |
|      | 331.1902  | 383.714   | 445.9593  |
|      | 513.5623  | 567.3083  | 644.9929  |
|      | 714.5256  | 797.9069  | 857.6302  |
|      | 946.3646  | 999.2914  | 1038.9843 |
|      | 1112.0205 | 1165.2182 | 1259.1578 |
|      | 1289.0164 | 1304.9585 | 1430.7785 |
|      | 1452.038  | 1483.124  | 1533.8399 |
|      | 1910.0253 | 2721.2767 | 3028.6769 |
|      | 3069.2695 | 3201.5924 | 3269.5599 |
|      | 3320.0529 | 3325.7646 | 3915.1218 |
| Pa1  | 57.1265   | 125.6681  | 126.1354  |
|      | 242.3745  | 348.7965  | 365.9529  |
|      | 533.2133  | 541.9714  | 619.0281  |
|      | 704.1106  | 928.357   | 967.8078  |
|      | 1021.02   | 1074.6894 | 1149.9969 |
|      | 1310.8627 | 1400.2875 | 1412.7128 |
|      | 1478.6802 | 1479.4919 | 1483.3877 |
|      | 1487.4408 | 1757.4592 | 1757.5023 |
|      | 3091.2507 | 3091.2611 | 3175.3084 |
|      | 3175.3284 | 3213.3676 | 3213.7714 |
| Pa2  | 469.018   | 757.8033  | 968.2392  |
|      | 1388.6971 | 1813.8115 | 3112.5528 |
| Pa3  | 56.1899   | 179.4841  | 221.4851  |
|      | 393.2576  | 478.1005  | 532.5618  |
|      | 758.2444  | 847.2178  | 876.5269  |
|      | 1022.0239 | 1061.4692 | 1206.3923 |
|      | 1267.6635 | 1327.1299 | 1408.4992 |
|      | 1471.842  | 1481.9293 | 1497.3453 |

|     |           |           |           |
|-----|-----------|-----------|-----------|
|     | 1780.4816 | 3090.3108 | 3117.9269 |
|     | 3175.8836 | 3207.0327 | 3211.0556 |
| Pa4 | 1211.5163 | 1290.595  | 1567.1527 |
|     | 1776.2605 | 2963.8158 | 3029.9251 |
| Pa5 | 49.9747   | 96.8945   | 130.0857  |
|     | 174.3619  | 209.5894  | 227.2532  |
|     | 274.3273  | 299.5832  | 354.431   |
|     | 400.0802  | 422.9367  | 496.4281  |
|     | 541.4043  | 624.2712  | 644.8667  |
|     | 694.2958  | 825.176   | 900.2923  |
|     | 967.5059  | 979.4566  | 1014.3948 |
|     | 1116.2132 | 1190.7133 | 1204.5395 |
|     | 1213.4167 | 1301.2591 | 1357.8361 |
|     | 1377.6948 | 1411.1444 | 1456.7117 |
|     | 1496.5255 | 1504.2095 | 1515.8489 |
|     | 1741.7337 | 1747.4125 | 3019.086  |
|     | 3095.7324 | 3131.8011 | 3191.9191 |
|     | 3205.3297 | 3206.3612 | 3822.8821 |
| Pb1 | 56.0093   | 63.3963   | 143.4008  |
|     | 190.8917  | 252.7658  | 259.915   |
|     | 281.5278  | 316.235   | 347.0975  |
|     | 433.8466  | 441.0731  | 566.3648  |
|     | 597.5377  | 731.3284  | 789.2104  |
|     | 915.2129  | 971.5308  | 1022.7057 |
|     | 1050.3671 | 1121.2076 | 1144.9251 |
|     | 1208.5805 | 1279.1544 | 1402.9582 |
|     | 1419.6044 | 1437.6075 | 1485.7678 |
|     | 1497.1892 | 1499.6543 | 1501.3036 |
|     | 1757.6632 | 1781.2015 | 2989.261  |
|     | 3080.5779 | 3102.1675 | 3172.3568 |
|     | 3198.0833 | 3211.5532 | 3212.1043 |
| Pb2 | 163.6459  | 352.2032  | 450.555   |
|     | 524.9367  | 616.9072  | 981.4444  |
|     | 1055.8614 | 1136.0794 | 1408.4556 |
|     | 1481.3625 | 1491.6475 | 1868.8963 |
|     | 3099.7639 | 3194.0596 | 3217.7189 |
| Pb3 | 47.5051   | 145.0389  | 219.9702  |
|     | 339.5067  | 367.8695  | 455.2881  |
|     | 561.6204  | 601.762   | 664.2502  |
|     | 901.8229  | 1030.6738 | 1042.3264 |
|     | 1234.4987 | 1408.2253 | 1477.6926 |
|     | 1486.3274 | 1775.3754 | 1801.9981 |
|     | 3092.8128 | 3177.6059 | 3218.2733 |
| Pb4 | 36.3975   | 78.3986   | 98.1919   |
|     | 166.8924  | 208.382   | 248.6032  |
|     | 273.5127  | 305.7829  | 326.5962  |
|     | 341.761   | 357.3376  | 411.2738  |
|     | 472.6926  | 534.5924  | 625.1159  |
|     | 791.7885  | 855.9594  | 917.9664  |



|     |           |           |           |
|-----|-----------|-----------|-----------|
|     | 973.0539  | 1002.3815 | 1068.74   |
|     | 1104.1148 | 1115.584  | 1179.9638 |
|     | 1235.0686 | 1320.605  | 1396.2762 |
|     | 1419.5874 | 1428.2234 | 1439.6298 |
|     | 1499.0727 | 1506.5243 | 1524.7268 |
|     | 1742.4425 | 1765.6278 | 3018.8977 |
|     | 3071.2893 | 3086.1924 | 3175.3845 |
|     | 3177.6209 | 3197.9367 | 3900.6984 |
| Pc1 | 39.3348   | 112.422   | 162.1727  |
|     | 225.9069  | 319.229   | 337.1729  |
|     | 390.0592  | 513.8129  | 570.8797  |
|     | 605.5187  | 725.8227  | 817.097   |
|     | 931.3948  | 970.5195  | 991.5515  |
|     | 1033.3612 | 1053.2941 | 1143.7343 |
|     | 1335.1703 | 1404.6714 | 1426.699  |
|     | 1441.8689 | 1493.6259 | 1497.6011 |
|     | 1670.1888 | 1748.7414 | 1759.6226 |
|     | 3061.8254 | 3084.2754 | 3170.4768 |
|     | 3186.3637 | 3207.1599 | 3291.7461 |
| TS1 | -416.7003 | 38.2998   | 110.4204  |
|     | 152.4616  | 163.6181  | 172.7389  |
|     | 274.7583  | 324.0125  | 378.2768  |
|     | 449.4052  | 573.0672  | 604.7756  |
|     | 711.4753  | 853.3512  | 943.9448  |
|     | 992.2976  | 1036.8541 | 1048.3778 |
|     | 1053.0264 | 1085.8636 | 1181.3373 |
|     | 1350.2525 | 1400.4148 | 1421.6452 |
|     | 1450.2023 | 1475.1801 | 1489.0195 |
|     | 1498.0886 | 1503.2336 | 1673.0334 |
|     | 2389.6136 | 3087.0135 | 3089.5753 |
|     | 3168.1255 | 3182.1803 | 3204.2905 |
|     | 3207.6626 | 3220.197  | 3311.7578 |
| TS2 | -430.145  | 70.2752   | 140.738   |
|     | 155.612   | 227.398   | 249.3913  |
|     | 280.9209  | 284.0297  | 372.2046  |
|     | 444.1353  | 545.9514  | 584.0164  |
|     | 684.0995  | 702.2437  | 937.9505  |
|     | 988.613   | 1001.7125 | 1046.6786 |
|     | 1050.1184 | 1076.5355 | 1176.6923 |
|     | 1354.5681 | 1402.5786 | 1422.9411 |
|     | 1458.9646 | 1482.3421 | 1490.0151 |
|     | 1502.8313 | 1506.7153 | 1628.7571 |
|     | 2323.5712 | 3088.7822 | 3092.606  |
|     | 3182.6746 | 3183.2134 | 3210.3323 |
|     | 3215.357  | 3220.6028 | 3324.3038 |
| TS3 | -678.9003 | 6.543     | 86.6378   |
|     | 111.8077  | 214.3472  | 222.47    |
|     | 271.3963  | 343.3439  | 354.3396  |
|     | 456.1183  | 522.1221  | 539.3482  |

|      |            |           |           |
|------|------------|-----------|-----------|
|      | 624.6562   | 640.9145  | 703.0012  |
|      | 898.4719   | 964.0163  | 1009.8505 |
|      | 1029.0305  | 1059.8789 | 1094.4254 |
|      | 1102.8637  | 1172.1179 | 1315.2348 |
|      | 1403.4771  | 1411.4897 | 1488.0657 |
|      | 1490.3798  | 1494.7825 | 1497.7705 |
|      | 1975.7207  | 2425.8067 | 3091.9838 |
|      | 3098.2733  | 3183.7362 | 3191.3911 |
|      | 3203.3691  | 3219.0788 | 3254.7229 |
| TS4  | -466.5682  | 23.6029   | 64.4002   |
|      | 80.1084    | 146.213   | 187.6299  |
|      | 251.8354   | 348.7013  | 354.2207  |
|      | 445.4533   | 509.1188  | 565.796   |
|      | 620.5858   | 667.5187  | 749.4126  |
|      | 879.0289   | 936.6704  | 971.4456  |
|      | 1038.3788  | 1055.7226 | 1105.6339 |
|      | 1134.8365  | 1232.9353 | 1276.0203 |
|      | 1395.7979  | 1423.6814 | 1485.7838 |
|      | 1495.4146  | 1497.944  | 1500.8596 |
|      | 1984.2651  | 2375.3457 | 3090.4846 |
|      | 3097.2631  | 3180.5167 | 3181.4183 |
|      | 3216.6788  | 3218.79   | 3292.3995 |
| TS5  | -1149.1768 | 40.517    | 61.1146   |
|      | 111.8987   | 188.8105  | 237.1578  |
|      | 321.2302   | 329.0378  | 381.2039  |
|      | 412.4225   | 472.2341  | 580.453   |
|      | 631.0937   | 712.4425  | 807.4898  |
|      | 948.441    | 964.741   | 970.6914  |
|      | 1021.3901  | 1081.2406 | 1090.0241 |
|      | 1115.5955  | 1140.6497 | 1178.0798 |
|      | 1368.3441  | 1429.8658 | 1433.5309 |
|      | 1490.3983  | 1493.9038 | 1513.2791 |
|      | 2194.4666  | 3084.5028 | 3141.295  |
|      | 3156.4328  | 3168.9302 | 3191.1819 |
|      | 3256.8882  | 3287.1377 | 4256.1319 |
| TS6  | -1457.4517 | 26.0372   | 42.2991   |
|      | 82.0091    | 152.3021  | 283.9896  |
|      | 336.0322   | 373.6347  | 395.9085  |
|      | 439.2897   | 480.7523  | 573.4239  |
|      | 619.9753   | 719.852   | 781.6272  |
|      | 933.7405   | 973.813   | 988.5005  |
|      | 1039.6152  | 1080.7643 | 1101.3104 |
|      | 1143.6666  | 1178.8329 | 1253.9435 |
|      | 1353.7555  | 1402.4022 | 1462.9425 |
|      | 1480.877   | 1491.9747 | 1500.3238 |
|      | 1776.4545  | 2405.276  | 3089.5034 |
|      | 3151.2526  | 3178.2007 | 3198.7152 |
|      | 3216.5649  | 3256.5657 | 3295.5352 |
| TSa1 | -702.8089  | 43.8672   | 59.0334   |

|      |            |           |           |
|------|------------|-----------|-----------|
|      | 76.1104    | 100.0177  | 124.7296  |
|      | 154.9865   | 162.641   | 205.0217  |
|      | 252.9113   | 281.1399  | 309.8809  |
|      | 332.3272   | 367.4179  | 410.0553  |
|      | 499.6488   | 529.7136  | 558.5664  |
|      | 637.5406   | 687.6269  | 702.2412  |
|      | 814.37     | 896.0195  | 935.3204  |
|      | 947.6669   | 999.0343  | 1040.9933 |
|      | 1044.3748  | 1127.8246 | 1159.0238 |
|      | 1201.8744  | 1255.7488 | 1327.5682 |
|      | 1345.3534  | 1394.3025 | 1419.4517 |
|      | 1483.5437  | 1493.4046 | 1499.5543 |
|      | 1506.5969  | 1515.7486 | 1670.7318 |
|      | 1769.3871  | 3082.98   | 3088.6335 |
|      | 3138.0545  | 3173.9092 | 3181.1686 |
|      | 3195.5236  | 3207.9641 | 3212.373  |
| TSa2 | -715.0026  | 46.924    | 98.8034   |
|      | 108.9113   | 149.7223  | 195.7983  |
|      | 210.9879   | 239.869   | 301.5777  |
|      | 349.5559   | 397.2452  | 531.6609  |
|      | 545.3289   | 569.8953  | 674.4582  |
|      | 718.9469   | 805.7395  | 918.9301  |
|      | 970.7503   | 1014.8613 | 1024.9769 |
|      | 1105.4462  | 1120.1322 | 1143.0996 |
|      | 1265.7373  | 1397.8504 | 1402.7535 |
|      | 1463.6193  | 1475.7571 | 1482.1197 |
|      | 1488.0097  | 1494.094  | 1618.5202 |
|      | 1973.0763  | 3090.6314 | 3092.1802 |
|      | 3179.9687  | 3180.2459 | 3192.5367 |
|      | 3215.6992  | 3222.5554 | 3320.3546 |
| TSa3 | -746.9902  | 55.0052   | 103.8266  |
|      | 196.1994   | 284.2265  | 408.8037  |
|      | 570.2931   | 681.0849  | 723.2961  |
|      | 972.7627   | 1045.4418 | 1120.1768 |
|      | 1258.0041  | 1380.34   | 1448.7218 |
|      | 1669.6849  | 3079.269  | 3151.3748 |
| TSa4 | -1338.4472 | 129.6331  | 230.2017  |
|      | 329.9671   | 432.316   | 609.8208  |
|      | 705.0965   | 756.6468  | 987.336   |
|      | 1259.5421  | 1303.2789 | 1485.8052 |
|      | 1884.9819  | 1938.6443 | 3048.7836 |
| TSa5 | -457.8579  | 75.208    | 109.6459  |
|      | 139.5535   | 173.7564  | 209.6432  |
|      | 245.7069   | 262.6072  | 322.0533  |
|      | 355.8783   | 395.3734  | 488.8523  |
|      | 524.5389   | 550.6457  | 760.7236  |
|      | 832.6114   | 881.9022  | 905.8713  |
|      | 994.5632   | 1027.8799 | 1054.902  |

|       |            |           |           |
|-------|------------|-----------|-----------|
|       | 1097.3995  | 1179.8853 | 1232.134  |
|       | 1314.8174  | 1368.2367 | 1404.8637 |
|       | 1440.6907  | 1475.6254 | 1486.9393 |
|       | 1496.2036  | 1502.1889 | 1507.5833 |
|       | 1967.8022  | 3089.0162 | 3097.1847 |
|       | 3124.7128  | 3183.451  | 3199.5999 |
|       | 3206.923   | 3210.8673 | 3228.5855 |
| TSa6  | -526.5561  | 40.0993   | 279.9239  |
|       | 551.0903   | 617.66    | 937.9878  |
|       | 1450.7149  | 1458.5788 | 2034.9998 |
|       | 3138.2523  | 3305.5759 | 3323.8049 |
| TSa7  | -698.5382  | 9.5553    | 159.042   |
|       | 190.0748   | 268.9197  | 542.9834  |
|       | 655.4952   | 1067.9611 | 1134.9943 |
|       | 1191.6577  | 1193.8949 | 1457.9235 |
|       | 1462.6862  | 1540.3508 | 1734.5522 |
|       | 2997.253   | 3068.7182 | 3077.5571 |
| TSa8  | -2080.2934 | 294.2728  | 359.0367  |
|       | 598.6994   | 602.0763  | 741.4409  |
|       | 1207.6123  | 1220.0506 | 1419.516  |
|       | 1500.8895  | 1566.8179 | 1770.7773 |
|       | 1821.6979  | 2979.4896 | 3062.4547 |
| TSa9  | -2319.0676 | 59.0589   | 91.5317   |
|       | 165.85     | 210.7799  | 238.7315  |
|       | 296.5917   | 312.7071  | 367.5401  |
|       | 408.0846   | 507.7164  | 541.5518  |
|       | 645.7926   | 653.933   | 688.5197  |
|       | 827.8236   | 870.0101  | 942.0015  |
|       | 976.29     | 1011.0129 | 1098.1128 |
|       | 1100.3437  | 1159.5367 | 1168.4635 |
|       | 1237.5023  | 1245.8115 | 1317.814  |
|       | 1347.5536  | 1415.0281 | 1436.061  |
|       | 1488.2898  | 1504.0095 | 1509.4617 |
|       | 1799.6073  | 1904.3732 | 3085.6042 |
|       | 3119.3546  | 3134.1981 | 3181.0463 |
|       | 3189.9098  | 3194.3942 | 3231.191  |
| TSa10 | -687.2081  | 19.2138   | 37.9795   |
|       | 60.5526    | 87.5436   | 96.9803   |
|       | 127.4337   | 172.078   | 201.2731  |
|       | 223.1919   | 257.3019  | 273.6115  |
|       | 301.3679   | 347.6174  | 379.147   |
|       | 422.2871   | 491.0248  | 539.5085  |
|       | 574.5355   | 643.0121  | 659.4724  |
|       | 678.4511   | 725.2508  | 829.4855  |
|       | 878.7259   | 954.6169  | 971.4159  |
|       | 1003.9747  | 1026.5512 | 1042.4675 |
|       | 1120.0851  | 1187.5242 | 1195.739  |
|       | 1212.7242  | 1257.1916 | 1301.8152 |
|       | 1339.3703  | 1356.9025 | 1412.383  |

|       |            |           |           |
|-------|------------|-----------|-----------|
|       | 1463.0608  | 1489.6339 | 1504.0777 |
|       | 1514.4219  | 1514.9559 | 1642.9226 |
|       | 1774.7438  | 3037.69   | 3093.5783 |
|       | 3120.1122  | 3121.1554 | 3185.2509 |
|       | 3195.1933  | 3212.1901 | 3759.7571 |
| TSa11 | -1777.5981 | 52.3881   | 78.2022   |
|       | 96.2825    | 125.8699  | 178.6405  |
|       | 190.0842   | 220.8791  | 241.2869  |
|       | 282.8015   | 297.6392  | 329.7539  |
|       | 360.6356   | 408.828   | 418.3721  |
|       | 455.3937   | 542.3621  | 583.3872  |
|       | 614.6355   | 663.9872  | 720.0926  |
|       | 747.1053   | 817.7236  | 898.3624  |
|       | 961.3859   | 979.3359  | 999.7209  |
|       | 1093.2882  | 1170.1303 | 1194.5939 |
|       | 1216.3075  | 1285.8105 | 1324.1344 |
|       | 1357.1508  | 1368.2735 | 1410.2134 |
|       | 1455.5788  | 1500.8516 | 1504.3783 |
|       | 1517.0548  | 1545.292  | 1782.7499 |
|       | 1887.7048  | 2637.9305 | 2967.6365 |
|       | 3096.0601  | 3133.4937 | 3193.7098 |
|       | 3205.5132  | 3208.9278 | 3804.5664 |
| TSb1  | -713.2993  | 27.0223   | 51.8495   |
|       | 68.2654    | 114.2094  | 129.3233  |
|       | 185.5184   | 205.2678  | 220.5377  |
|       | 246.9586   | 271.4114  | 300.7634  |
|       | 309.2006   | 362.2184  | 381.5302  |
|       | 465.5494   | 531.6942  | 565.9963  |
|       | 591.3138   | 675.0779  | 719.7822  |
|       | 807.535    | 935.5672  | 990.1237  |
|       | 998.2192   | 1054.1571 | 1077.0379 |
|       | 1094.9434  | 1128.6878 | 1166.5217 |
|       | 1232.0857  | 1243.8557 | 1327.5359 |
|       | 1379.4484  | 1398.3422 | 1426.2668 |
|       | 1493.6387  | 1496.7428 | 1501.8935 |
|       | 1503.6089  | 1545.8822 | 1689.4548 |
|       | 1773.2461  | 3035.3067 | 3084.5964 |
|       | 3091.0831  | 3092.8919 | 3175.7885 |
|       | 3187.1268  | 3204.4728 | 3205.0249 |
| TSb2  | -1723.9914 | 50.0293   | 56.8284   |
|       | 109.7967   | 158.2085  | 170.8158  |
|       | 185.853    | 237.046   | 265.7327  |
|       | 280.5127   | 319.396   | 333.347   |
|       | 356.3284   | 421.2698  | 466.8767  |
|       | 555.3529   | 587.5932  | 641.1698  |
|       | 705.7358   | 764.9346  | 809.8592  |
|       | 921.219    | 964.0112  | 996.6278  |
|       | 1047.0854  | 1118.4557 | 1145.8297 |
|       | 1205.3671  | 1272.8923 | 1324.329  |

|      |           |           |           |
|------|-----------|-----------|-----------|
|      | 1384.0609 | 1403.0735 | 1427.6278 |
|      | 1488.1586 | 1497.2513 | 1501.2565 |
|      | 1503.1021 | 1523.7079 | 1772.3113 |
|      | 1811.8724 | 1873.8085 | 2970.6049 |
|      | 3085.9136 | 3094.079  | 3175.8533 |
|      | 3186.7554 | 3207.5556 | 3208.9726 |
|      | 3187.1268 | 3204.4728 | 3205.0249 |
| TSb3 | -656.4519 | 67.5327   | 138.0778  |
|      | 162.5331  | 193.625   | 200.6981  |
|      | 239.4512  | 262.5869  | 285.8103  |
|      | 323.6247  | 368.8858  | 434.9289  |
|      | 494.7882  | 581.7239  | 656.6742  |
|      | 715.9335  | 854.2996  | 991.7031  |
|      | 1015.4709 | 1050.601  | 1138.4785 |
|      | 1154.7861 | 1210.8708 | 1285.4084 |
|      | 1294.7768 | 1398.481  | 1415.3206 |
|      | 1481.7678 | 1492.4167 | 1494.9201 |
|      | 1501.1096 | 1536.3189 | 1678.6454 |
|      | 2209.7983 | 2940.0219 | 3012.2763 |
|      | 3084.4318 | 3091.6391 | 3176.2225 |
|      | 3186.8853 | 3207.7281 | 3214.5339 |
| TSb4 | -708.4459 | 46.5776   | 62.2508   |
|      | 75.9989   | 140.3614  | 150.293   |
|      | 166.9895  | 206.4163  | 271.0933  |
|      | 287.708   | 314.9474  | 351.1896  |
|      | 383.3295  | 495.3445  | 514.742   |
|      | 562.0946  | 577.3604  | 676.2103  |
|      | 692.0609  | 789.5847  | 936.1737  |
|      | 1006.7752 | 1024.6167 | 1038.368  |
|      | 1111.1142 | 1147.4901 | 1236.2788 |
|      | 1292.9491 | 1406.6978 | 1421.0942 |
|      | 1480.5695 | 1489.7268 | 1493.8063 |
|      | 1506.8752 | 1664.9864 | 1775.7593 |
|      | 3092.3541 | 3092.9481 | 3181.4625 |
|      | 3184.0148 | 3214.4713 | 3215.1089 |
| TSb5 | -645.6359 | 67.3237   | 148.0815  |
|      | 181.3304  | 243.7412  | 251.8671  |
|      | 305.3216  | 339.1319  | 381.7325  |
|      | 434.4091  | 530.084   | 544.9101  |
|      | 632.5792  | 843.01    | 974.5707  |
|      | 1040.6996 | 1048.791  | 1091.7369 |
|      | 1126.091  | 1296.5349 | 1394.2221 |
|      | 1408.0367 | 1471.8857 | 1490.7352 |
|      | 1492.2059 | 1496.1364 | 1898.3658 |
|      | 3097.0714 | 3099.7583 | 3196.3905 |
|      | 3201.6898 | 3217.6783 | 3227.4784 |
| TSb6 | -583.3626 | 49.2572   | 144.6692  |
|      | 181.7239  | 200.293   | 233.9675  |
|      | 249.1457  | 320.3479  | 411.5038  |

|      |            |           |           |
|------|------------|-----------|-----------|
|      | 415.4761   | 541.3777  | 568.454   |
|      | 584.2676   | 671.6017  | 704.3736  |
|      | 861.0959   | 1000.9465 | 1037.2646 |
|      | 1089.6441  | 1188.4807 | 1400.5673 |
|      | 1447.7979  | 1456.2613 | 1474.04   |
|      | 1482.7804  | 1790.0668 | 1832.3334 |
|      | 3093.7048  | 3136.9104 | 3181.9471 |
|      | 3217.8362  | 3316.3706 | 3330.6113 |
| TSb7 | -2415.7768 | 62.3075   | 129.96    |
|      | 187.9653   | 208.0091  | 256.3621  |
|      | 287.5163   | 372.2041  | 431.1401  |
|      | 451.5979   | 478.612   | 561.5247  |
|      | 575.5311   | 655.6728  | 721.0986  |
|      | 860.6652   | 973.8738  | 995.1403  |
|      | 1006.3859  | 1052.9081 | 1062.1061 |
|      | 1137.9092  | 1157.0036 | 1198.1467 |
|      | 1216.753   | 1253.3632 | 1307.1598 |
|      | 1370.9793  | 1401.6812 | 1457.4005 |
|      | 1487.2023  | 1501.9379 | 1534.6522 |
|      | 1778.7086  | 1869.1367 | 3063.7666 |
|      | 3084.8425  | 3147.3497 | 3150.1938 |
|      | 3175.6333  | 3209.6427 | 3257.6479 |
| TSb8 | -2223.2763 | 79.2086   | 168.8167  |
|      | 188.7349   | 245.0046  | 277.4806  |
|      | 321.793    | 329.8102  | 361.7595  |
|      | 451.8084   | 474.3898  | 559.166   |
|      | 615.3387   | 639.6377  | 737.9317  |
|      | 791.7657   | 928.2011  | 1005.5515 |
|      | 1017.2428  | 1085.1256 | 1110.5378 |
|      | 1134.9463  | 1147.8977 | 1215.0308 |
|      | 1230.0411  | 1252.2532 | 1299.5374 |
|      | 1394.5314  | 1428.3108 | 1435.3635 |
|      | 1491.7692  | 1502.0092 | 1503.1738 |
|      | 1588.635   | 2098.8516 | 3024.5078 |
|      | 3087.6938  | 3105.0118 | 3141.7827 |
|      | 3179.3792  | 3199.1684 | 3237.6118 |
| TSb9 | -694.7024  | 19.3921   | 32.0364   |
|      | 39.1514    | 89.0735   | 93.4023   |
|      | 138.2058   | 190.173   | 209.241   |
|      | 215.8311   | 244.4935  | 273.9991  |
|      | 279.8899   | 318.5936  | 338.9505  |
|      | 359.1945   | 422.8411  | 460.8251  |
|      | 528.6624   | 552.3851  | 629.504   |
|      | 686.2363   | 791.7534  | 823.8344  |
|      | 930.6556   | 972.6405  | 1010.2384 |
|      | 1072.1631  | 1083.3659 | 1107.1888 |
|      | 1119.534   | 1128.1485 | 1194.3502 |
|      | 1223.5326  | 1251.5926 | 1315.6178 |
|      | 1366.8856  | 1397.3837 | 1422.9156 |

|       |            |           |           |
|-------|------------|-----------|-----------|
|       | 1434.4283  | 1499.0598 | 1508.2023 |
|       | 1519.5752  | 1536.3324 | 1675.6816 |
|       | 1754.0381  | 3034.4817 | 3065.6492 |
|       | 3086.4068  | 3097.3094 | 3167.4197 |
|       | 3181.5871  | 3191.8272 | 3901.086  |
| Tsb10 | -2095.9844 | 27.8435   | 46.6321   |
|       | 81.5498    | 110.9615  | 151.9659  |
|       | 189.7969   | 223.1286  | 245.8236  |
|       | 269.6851   | 303.0533  | 325.7742  |
|       | 337.1365   | 347.8402  | 381.1883  |
|       | 405.5836   | 465.526   | 536.771   |
|       | 640.6478   | 716.7808  | 742.2781  |
|       | 769.61     | 860.2788  | 927.3677  |
|       | 957.4991   | 1001.9709 | 1069.9111 |
|       | 1104.4843  | 1113.6344 | 1174.8289 |
|       | 1235.9698  | 1311.2945 | 1353.8415 |
|       | 1389.0089  | 1397.7466 | 1423.4504 |
|       | 1434.7286  | 1497.403  | 1505.4158 |
|       | 1521.3329  | 1533.4999 | 1744.5346 |
|       | 1812.4569  | 2527.2466 | 3027.6769 |
|       | 3068.6454  | 3086.3625 | 3178.234  |
|       | 3179.9698  | 3198.85   | 3899.5761 |
| TSc1  | -709.2291  | 20.299    | 36.7923   |
|       | 48.8832    | 84.924    | 123.8721  |
|       | 157.8328   | 198.9556  | 238.6243  |
|       | 284.5738   | 378.4622  | 411.7481  |
|       | 463.5103   | 565.1811  | 573.469   |
|       | 637.9995   | 700.3391  | 721.1305  |
|       | 737.7325   | 922.9246  | 959.4514  |
|       | 979.123    | 1043.821  | 1050.4176 |
|       | 1098.7908  | 1118.1462 | 1172.7552 |
|       | 1258.3465  | 1347.9321 | 1382.9046 |
|       | 1405.3466  | 1455.0852 | 1492.2129 |
|       | 1498.6535  | 1527.1796 | 1677.4677 |
|       | 1725.0126  | 1745.9804 | 3012.6636 |
|       | 3083.9952  | 3084.8476 | 3170.2441 |
|       | 3182.2673  | 3204.7223 | 3278.4732 |
| TSc2  | -1950.1591 | 36.2041   | 52.0289   |
|       | 117.5052   | 141.6029  | 182.3474  |
|       | 270.0303   | 313.2156  | 323.2391  |
|       | 368.5415   | 394.3212  | 512.2958  |
|       | 581.7419   | 600.4056  | 678.0428  |
|       | 758.0812   | 801.031   | 856.6474  |
|       | 918.5318   | 998.7722  | 1030.6602 |
|       | 1086.5323  | 1155.2832 | 1169.5211 |
|       | 1341.5469  | 1346.2096 | 1377.7168 |
|       | 1402.2472  | 1479.3218 | 1487.2867 |
|       | 1497.0714  | 1498.0785 | 1823.0424 |
|       | 1913.3061  | 2123.2794 | 2955.119  |



|      |            |           |           |
|------|------------|-----------|-----------|
|      | 3083.623   | 3098.2452 | 3178.1002 |
|      | 3212.2459  | 3275.2171 | 3681.3482 |
| TSc3 | -532.0291  | 33.4759   | 66.2729   |
|      | 139.8077   | 160.2487  | 194.0017  |
|      | 242.0079   | 291.5627  | 456.1485  |
|      | 533.1972   | 595.8238  | 679.4289  |
|      | 683.3806   | 741.1507  | 966.3695  |
|      | 1015.5555  | 1073.8601 | 1079.0385 |
|      | 1190.5049  | 1241.2123 | 1289.2566 |
|      | 1407.658   | 1428.5376 | 1477.8214 |
|      | 1484.9869  | 1553.2766 | 1781.4584 |
|      | 2077.9203  | 2397.6123 | 2919.0139 |
|      | 2991.4994  | 3086.9732 | 3155.695  |
|      | 3175.6518  | 3218.5912 | 3259.5377 |
| TSc4 | -2255.0463 | 68.2581   | 161.2896  |
|      | 286.6423   | 331.3513  | 377.5899  |
|      | 469.8764   | 491.6674  | 538.9363  |
|      | 615.7174   | 708.675   | 729.6116  |
|      | 759.1827   | 914.9111  | 940.4887  |
|      | 1002.5071  | 1038.4551 | 1065.7258 |
|      | 1096.9937  | 1148.3055 | 1234.246  |
|      | 1265.6688  | 1314.1335 | 1385.2568 |
|      | 1431.814   | 1449.6713 | 1498.9879 |
|      | 1618.2466  | 1748.8384 | 1948.0294 |
|      | 3030.4929  | 3110.6055 | 3124.2186 |
|      | 3185.9499  | 3225.6055 | 3284.7866 |

**Table S3** T1 diagnostic values of various species involved in the reaction of MIK with Cl atoms.

| Species         | T1 diag | Species | T1 diag | Species | T1 diag |
|-----------------|---------|---------|---------|---------|---------|
| MIK             | 0.014   | IMa7    | 0.018   | IMb4    | 0.020   |
| Cl              | 0.006   | TSa4    | 0.037   | IMb5    | 0.022   |
| IM01            | 0.014   | Pa2     | 0.017   | IMb6    | 0.020   |
| TS1             | 0.022   | TSa5    | 0.024   | TSb4    | 0.026   |
| IM1             | 0.018   | Pa3     | 0.014   | IMb7    | 0.023   |
| TS2             | 0.022   | IMa8    | 0.021   | TSb5    | 0.030   |
| IM2             | 0.014   | TSa6    | 0.022   | Pb2     | 0.015   |
| TS3             | 0.025   | IMa9    | 0.008   | TSb6    | 0.023   |
| IM3             | 0.028   | CO      | 0.021   | Pb3     | 0.016   |
| HCl             | 0.006   | IMa10   | 0.028   | TSb7    | 0.018   |
| TS4             | 0.026   | IMa11   | 0.023   | IMb8    | 0.017   |
| IM4             | 0.028   | TSa7    | 0.037   | IMb9    | 0.020   |
| TS5             | 0.018   | IMa12   | 0.017   | IMb10   | 0.018   |
| IM5             | 0.015   | TSa8    | 0.041   | TSb8    | 0.025   |
| TS6             | 0.024   | Pa4     | 0.017   | IMb11   | 0.016   |
| IM6             | 0.025   | TSa9    | 0.022   | TSb9    | 0.034   |
| O <sub>2</sub>  | 0.018   | IMa13   | 0.018   | Pb4     | 0.014   |
| IMa1            | 0.021   | IMa14   | 0.020   | TSb10   | 0.018   |
| NO              | 0.023   | IMa15   | 0.019   | IMb12   | 0.014   |
| IMa2            | 0.019   | TSa10   | 0.024   | IMc1    | 0.022   |
| NO <sub>2</sub> | 0.026   | IMa16   | 0.022   | IMc2    | 0.020   |
| TSa1            | 0.017   | TSa11   | 0.028   | TSa1    | 0.029   |
| IMa3            | 0.026   | Pa5     | 0.015   | IMc3    | 0.017   |
| TSa2            | 0.024   | IMb1    | 0.020   | TSa2    | 0.032   |
| IMa4            | 0.015   | IMb2    | 0.019   | Pc1     | 0.017   |
| Pa1             | 0.016   | TSb1    | 0.026   | TSa3    | 0.031   |
| HO <sub>2</sub> | 0.029   | IMb3    | 0.016   | IMc4    | 0.032   |
| IMa5            | 0.024   | TSb2    | 0.029   | TSa4    | 0.020   |
| IMa6            | 0.022   | Pb1     | 0.015   | IMc5    | 0.017   |
| TSa3            | 0.031   | TSb3    | 0.023   |         |         |

**Table S4** The overall rate constant of addition channels and the total rate constant for the reaction of MIK with Cl atoms at the temperature range of 180-380 K and 1atm.

| T (K) | ACR              |                  | MACR             |                  | MVK              |                  | MIK              |                  |
|-------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
|       | $k_{\text{add}}$ | $k_{\text{tot}}$ | $k_{\text{add}}$ | $k_{\text{tot}}$ | $k_{\text{add}}$ | $k_{\text{tot}}$ | $k_{\text{add}}$ | $k_{\text{tot}}$ |
| 180   | 2.38E-10         | 2.39E-10         | 8.98E-10         | 8.98E-10         | 5.15E-10         | 5.15E-10         | 2.79E-10         | 2.81E-10         |
| 200   | 2.29E-10         | 2.30E-10         | 7.32E-10         | 7.32E-10         | 6.96E-10         | 6.96E-10         | 2.66E-10         | 2.69E-10         |
| 220   | 2.22E-10         | 2.23E-10         | 6.66E-10         | 6.67E-10         | 3.80E-10         | 3.80E-10         | 2.58E-10         | 2.61E-10         |
| 240   | 2.15E-10         | 2.16E-10         | 5.07E-10         | 5.08E-10         | 3.24E-10         | 3.24E-10         | 2.39E-10         | 2.42E-10         |
| 260   | 2.10E-10         | 2.11E-10         | 3.72E-10         | 3.74E-10         | 2.67E-10         | 2.67E-10         | 2.23E-10         | 2.26E-10         |
| 280   | 2.01E-10         | 2.02E-10         | 3.02E-10         | 3.05E-10         | 2.13E-10         | 2.13E-10         | 1.96E-10         | 2.00E-10         |
| 298   | 1.94E-10         | 1.96E-10         | 2.38E-10         | 2.42E-10         | 1.59E-10         | 1.59E-10         | 1.82E-10         | 1.86E-10         |
| 320   | 1.87E-10         | 1.89E-10         | 6.24E-11         | 6.67E-11         | 1.21E-10         | 1.21E-10         | 1.53E-10         | 1.57E-10         |
| 340   | 1.89E-10         | 1.91E-10         | 4.53E-11         | 5.00E-11         | 8.62E-11         | 8.64E-11         | 1.32E-10         | 1.36E-10         |
| 360   | 1.93E-10         | 1.95E-10         | 2.73E-11         | 3.22E-11         | 6.07E-11         | 6.09E-11         | 1.12E-10         | 1.17E-10         |
| 380   | 1.99E-10         | 2.01E-10         | 2.95E-11         | 3.43E-11         | 3.62E-11         | 3.65E-11         | 1.00E-10         | 1.05E-10         |

**Table S5** Cartesian coordinates (bohr) for the optimized stationary points

| Optimized stationary points | Cartesian coordinates (bohr) |             |             |             |
|-----------------------------|------------------------------|-------------|-------------|-------------|
| MIK                         | C                            | -0.89888900 | 1.59294000  | -0.00017600 |
|                             | H                            | -0.07960900 | 2.30335600  | -0.00025400 |
|                             | H                            | -1.90582500 | 2.00006300  | -0.00017300 |
|                             | C                            | -0.69248200 | 0.26233100  | -0.00009700 |
|                             | C                            | 0.68995800  | -0.31822700 | -0.00013400 |
|                             | C                            | 1.88904200  | 0.61219300  | 0.00006800  |
|                             | H                            | 1.87725100  | 1.25525400  | 0.88457000  |
|                             | H                            | 2.79421000  | 0.00477100  | 0.00019100  |
|                             | H                            | 1.87752000  | 1.25530200  | -0.88439800 |
|                             | C                            | -1.81380600 | -0.73928100 | 0.00005900  |
|                             | H                            | -1.74319200 | -1.38827200 | -0.87699200 |
|                             | H                            | -1.74340500 | -1.38775300 | 0.87751700  |
|                             | H                            | -2.78415900 | -0.23731600 | -0.00019300 |
|                             | O                            | 0.83303400  | -1.53314200 | 0.00017700  |
| IM01                        | C                            | 0.60099700  | 0.14221900  | 1.53050600  |
|                             | H                            | 0.41881000  | -0.84240600 | 1.94481800  |
|                             | H                            | 1.37533900  | 0.74721600  | 1.99129000  |
|                             | C                            | -0.11800200 | 0.62543400  | 0.47413600  |
|                             | C                            | -1.26697900 | -0.15865800 | -0.11528600 |
|                             | C                            | -1.48801700 | -1.58878200 | 0.32764700  |
|                             | H                            | -1.76092600 | -1.61674600 | 1.38722800  |
|                             | H                            | -2.30101500 | -2.00816100 | -0.26490400 |
|                             | H                            | -0.58012900 | -2.18037300 | 0.18933900  |
|                             | C                            | 0.06078300  | 2.01819800  | -0.04752100 |
|                             | H                            | 0.10439700  | 2.01029400  | -1.13794700 |
|                             | H                            | -0.80469200 | 2.62433100  | 0.23780600  |
|                             | H                            | 0.97064500  | 2.47014100  | 0.35178200  |
|                             | O                            | -1.99954100 | 0.39298500  | -0.91749400 |
|                             | Cl                           | 1.87301200  | -0.62227300 | -0.61037400 |
| IM1                         | C                            | 0.97781200  | 0.06239300  | 0.89120800  |
|                             | H                            | 0.83973900  | -0.84865800 | 1.47079500  |
|                             | H                            | 1.49164600  | 0.81016700  | 1.49598200  |
|                             | C                            | -0.28642600 | 0.60249700  | 0.33596200  |
|                             | C                            | -1.42415100 | -0.28564700 | -0.04950400 |
|                             | C                            | -1.25227000 | -1.77261200 | 0.20460100  |
|                             | H                            | -1.20432900 | -1.96169200 | 1.28181500  |
|                             | H                            | -2.10985000 | -2.29457700 | -0.21765700 |
|                             | H                            | -0.32542900 | -2.13849000 | -0.24561100 |
|                             | C                            | -0.37163700 | 2.05221200  | 0.01313000  |
|                             | H                            | 0.40074600  | 2.32040300  | -0.71949900 |
|                             | H                            | -1.35344400 | 2.28715900  | -0.39684100 |
|                             | H                            | -0.19134400 | 2.65893000  | 0.90884000  |
|                             | O                            | -2.42316000 | 0.16813000  | -0.52996200 |
|                             | Cl                           | 2.11632800  | -0.36066700 | -0.45356000 |
| IM2                         | C                            | 0.54182800  | -0.04149200 | 1.73557700  |
|                             | H                            | 0.07046700  | -0.92281900 | 2.15034500  |
|                             | H                            | 1.31867700  | 0.45022300  | 2.30798200  |
|                             | C                            | 0.36798100  | 0.30111200  | 0.30702400  |
|                             | C                            | -1.10587700 | 0.18710800  | -0.13835600 |
|                             | C                            | -1.87170600 | -1.05727000 | 0.26022000  |
|                             | H                            | -2.27278700 | -0.90567500 | 1.26786500  |
|                             | H                            | -2.70721700 | -1.18661700 | -0.42853600 |
|                             | H                            | -1.24168700 | -1.94758000 | 0.26632400  |

|     |    |             |             |             |
|-----|----|-------------|-------------|-------------|
|     | C  | 0.95281800  | 1.65504600  | -0.05105100 |
|     | H  | 0.82782300  | 1.85556500  | -1.11493800 |
|     | H  | 0.42789500  | 2.43165900  | 0.51209100  |
|     | H  | 2.01509700  | 1.67601100  | 0.20264900  |
|     | O  | -1.62442300 | 1.09374400  | -0.75805400 |
|     | Cl | 1.24981400  | -0.96869100 | -0.69293200 |
| IM3 | C  | 0.85134500  | 1.60752000  | -0.11155600 |
|     | H  | 1.66387300  | 2.32055700  | -0.14646100 |
|     | C  | 0.70490000  | 0.33336200  | -0.00840800 |
|     | C  | -0.69310800 | -0.29780100 | -0.02955300 |
|     | C  | -1.87211200 | 0.64175400  | 0.09717900  |
|     | H  | -1.77569000 | 1.47316900  | -0.60468500 |
|     | H  | -2.79193500 | 0.08476900  | -0.08033700 |
|     | H  | -1.87701800 | 1.05999900  | 1.10809400  |
|     | C  | 1.83582100  | -0.66240300 | 0.10029000  |
|     | H  | 1.72755300  | -1.23997600 | 1.02232600  |
|     | H  | 1.77424200  | -1.36747900 | -0.73200200 |
|     | H  | 2.80636900  | -0.16344100 | 0.09245100  |
|     | O  | -0.81105800 | -1.48777400 | -0.11838700 |
| IM4 | C  | 0.73184800  | 1.69008000  | 0.00000600  |
|     | H  | 0.02791500  | 2.50912400  | 0.00002500  |
|     | C  | 0.70874600  | 0.40370100  | -0.00000400 |
|     | C  | -0.62990100 | -0.36384000 | 0.00000300  |
|     | C  | -1.90637600 | 0.45238300  | -0.00000600 |
|     | H  | -1.93564300 | 1.09323900  | -0.88512800 |
|     | H  | -2.75718800 | -0.22813600 | 0.00003600  |
|     | H  | -1.93562400 | 1.09332500  | 0.88505400  |
|     | C  | 1.92349700  | -0.48575700 | -0.00000700 |
|     | H  | 1.90248000  | -1.13548900 | 0.87862100  |
|     | H  | 1.90237100  | -1.13564500 | -0.87851500 |
|     | H  | 2.83878300  | 0.10711200  | -0.00011000 |
|     | O  | -0.62624700 | -1.56036600 | 0.00000800  |
| IM5 | C  | 0.84566600  | 1.57661600  | -0.00010400 |
|     | H  | -0.01600600 | 2.23983100  | -0.00010200 |
|     | H  | 1.83243300  | 2.03160100  | -0.00015800 |
|     | C  | 0.68469200  | 0.27726000  | 0.00002200  |
|     | C  | -0.72457100 | -0.29103100 | 0.00000400  |
|     | C  | -1.88007500 | 0.67745900  | 0.00011600  |
|     | H  | -2.42318400 | 0.80449600  | -0.92833100 |
|     | H  | -2.42314900 | 0.80430200  | 0.92860900  |
|     | C  | 1.78124900  | -0.74489100 | 0.00009500  |
|     | H  | 1.69070700  | -1.39210500 | 0.87685000  |
|     | H  | 1.69119000  | -1.39167600 | -0.87702100 |
|     | H  | 2.76308000  | -0.26635400 | 0.00048600  |
|     | O  | -0.91960500 | -1.47532100 | -0.00014200 |
| IM6 | C  | 1.16623400  | 1.43385600  | -0.09183200 |
|     | H  | 0.44990600  | 2.24002000  | -0.16985700 |
|     | H  | 2.21686000  | 1.70223600  | -0.09155900 |
|     | C  | 0.78888800  | 0.11371000  | -0.00136000 |
|     | C  | -0.69746700 | -0.28541800 | -0.02047100 |
|     | C  | -1.71907700 | 0.82781300  | 0.10468700  |
|     | H  | -1.65034500 | 1.49416900  | -0.76010700 |
|     | H  | -2.71226700 | 0.38244900  | 0.14837700  |
|     | H  | -1.52731700 | 1.42160600  | 1.00238400  |
|     | C  | 1.68504700  | -0.93381900 | 0.10272300  |
|     | H  | 1.32025700  | -1.95063400 | 0.15420900  |
|     | H  | 2.75278600  | -0.75131400 | 0.13057300  |
|     | O  | -1.02395500 | -1.43442300 | -0.12206400 |

|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
| IMa1 | C  | 0.92995600  | -0.70449300 | -0.85767700 |
|      | H  | 0.79392000  | -0.19249600 | -1.81089700 |
|      | H  | 1.08273400  | -1.77034300 | -1.03458900 |
|      | C  | -0.28889400 | -0.49589500 | 0.03593500  |
|      | C  | -0.47860400 | 0.99789800  | 0.37440200  |
|      | C  | -0.60484300 | 1.95217000  | -0.79264900 |
|      | H  | -1.15024700 | 1.50788700  | -1.62665500 |
|      | H  | -1.10247300 | 2.86073000  | -0.45212400 |
|      | H  | 0.40358900  | 2.21303400  | -1.13294700 |
|      | C  | -0.30277300 | -1.37067700 | 1.26841600  |
|      | H  | 0.53835100  | -1.11655500 | 1.91440500  |
|      | H  | -1.22722800 | -1.20373400 | 1.82186600  |
|      | H  | -0.23492700 | -2.42083400 | 0.97112500  |
|      | O  | -0.47771300 | 1.36411700  | 1.53053700  |
|      | Cl | 2.38953600  | -0.05338000 | -0.08246400 |
|      | O  | -1.38444800 | -0.90534000 | -0.85767400 |
|      | O  | -2.54470000 | -0.61430800 | -0.35022000 |
| IMa2 | C  | 1.10320100  | -0.94824700 | -0.84402400 |
|      | H  | 1.21691600  | -0.44894300 | -1.80632100 |
|      | H  | 0.75572000  | -1.97072100 | -0.99963400 |
|      | C  | 0.09963100  | -0.18848200 | 0.02572900  |
|      | C  | 0.62739100  | 1.22695600  | 0.34966300  |
|      | C  | 0.93139600  | 2.12373800  | -0.82926200 |
|      | H  | 0.20423100  | 1.98776900  | -1.63090000 |
|      | H  | 0.94263600  | 3.15992400  | -0.48937200 |
|      | H  | 1.92711500  | 1.87034500  | -1.21084900 |
|      | C  | -0.27996900 | -0.94240500 | 1.28343800  |
|      | H  | 0.59727500  | -1.07470700 | 1.91773900  |
|      | H  | -1.01434300 | -0.37105300 | 1.85341100  |
|      | H  | -0.68969200 | -1.91966400 | 1.01512000  |
|      | O  | 0.80408400  | 1.56652300  | 1.50208100  |
|      | Cl | 2.69836400  | -1.01519900 | -0.06252400 |
|      | O  | -1.00764600 | -0.07215700 | -0.89235100 |
|      | O  | -1.97289700 | 0.79372700  | -0.29917200 |
|      | N  | -3.21526100 | -0.06019600 | 0.12009500  |
|      | O  | -3.09793100 | -1.18591300 | -0.10308500 |
| IMa3 | C  | -0.98310200 | 0.40216500  | -0.87290500 |
|      | H  | -0.84036100 | -0.17413700 | -1.78782800 |
|      | H  | -1.48123400 | 1.34292500  | -1.11014400 |
|      | C  | 0.37009400  | 0.69401500  | -0.21331700 |
|      | C  | 1.04195800  | -0.59816600 | 0.31064500  |
|      | C  | 1.31559000  | -1.65728200 | -0.73469000 |
|      | H  | 1.70418400  | -1.20206600 | -1.64997100 |
|      | H  | 2.02681400  | -2.38199900 | -0.33737500 |
|      | H  | 0.37920200  | -2.17192000 | -0.97575200 |
|      | C  | 0.24857300  | 1.73635700  | 0.90399000  |
|      | H  | -0.40960900 | 1.33589500  | 1.67619100  |
|      | H  | 1.22786400  | 1.92663800  | 1.34278400  |
|      | H  | -0.16721000 | 2.66203700  | 0.49993100  |
|      | O  | 1.34245500  | -0.72730600 | 1.47944600  |
|      | Cl | -2.03788100 | -0.54396000 | 0.20524700  |
|      | O  | 1.18825100  | 1.28323300  | -1.16811700 |
| IMa4 | C  | -1.11696900 | 0.00000000  | -0.03224600 |
|      | H  | -1.61446600 | -0.94965300 | 0.07485000  |
|      | H  | -1.61443200 | 0.94966900  | 0.07484900  |
|      | Cl | 0.58416000  | -0.00000100 | 0.00257500  |
| IMa5 | O  | 1.16513300  | 0.31418300  | -0.45198400 |
|      | O  | 1.76708800  | -0.64184900 | 0.20031800  |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | C  | 0.01222900  | 0.76655100  | 0.25985000  |
|       | H  | 0.23670700  | 0.75901500  | 1.32350900  |
|       | H  | -0.18735700 | 1.76103600  | -0.13085400 |
|       | Cl | -1.38708700 | -0.26459000 | -0.04343700 |
| IMa6  | O  | -0.25072700 | 1.07219200  | 0.55589100  |
|       | O  | -1.06708100 | 0.88393200  | -0.59700100 |
|       | O  | -1.61034100 | -1.02666800 | 0.56576500  |
|       | N  | -1.85116900 | -0.48470500 | -0.41892300 |
|       | C  | 1.07356400  | 0.95021600  | 0.14417900  |
|       | H  | 1.24212600  | 1.49394100  | -0.78358700 |
|       | H  | 1.65732900  | 1.34427900  | 0.97444700  |
|       | Cl | 1.59073700  | -0.74013100 | -0.13651300 |
| IMa7  | O  | -1.58561400 | -0.43714900 | -0.00008600 |
|       | C  | -0.63392500 | 0.50575100  | -0.00007500 |
|       | H  | -0.75729100 | 1.13230700  | -0.89169300 |
|       | H  | -0.75801900 | 1.13088900  | 0.89275200  |
|       | Cl | 1.05904500  | -0.10591200 | 0.00000400  |
| IMa8  | C  | 0.24839600  | -0.44204100 | -0.00003200 |
|       | C  | -1.17093100 | 0.10026700  | -0.00000200 |
|       | H  | -1.68535000 | -0.28489500 | 0.88253000  |
|       | H  | -1.17009900 | 1.19386600  | -0.00062200 |
|       | H  | -1.68589900 | -0.28587100 | -0.88177900 |
|       | O  | 1.25956900  | 0.17844300  | 0.00000900  |
| IMa9  | C  | 0.00017800  | -0.00001900 | -0.00020200 |
|       | H  | -0.49313700 | 0.95976900  | 0.00040500  |
|       | H  | -0.58581600 | -0.90622900 | 0.00040500  |
|       | H  | 1.07788700  | -0.05342400 | 0.00040500  |
| IMa10 | O  | 0.16528600  | 0.54077300  | 0.00006400  |
|       | O  | 1.16705400  | -0.28007700 | -0.00004300 |
|       | C  | -1.08600600 | -0.17997500 | 0.00000900  |
|       | H  | -1.14196700 | -0.79542000 | 0.89758900  |
|       | H  | -1.85954700 | 0.58631700  | -0.00116800 |
|       | H  | -1.14117500 | -0.79661800 | -0.89664000 |
| IMa11 | O  | 0.79609700  | 0.18367700  | 0.63844700  |
|       | O  | -0.11834800 | 0.98403000  | -0.09916700 |
|       | O  | -1.40245000 | -0.83643100 | 0.14170300  |
|       | N  | -1.40520200 | 0.24664300  | -0.28927100 |
|       | C  | 1.66057700  | -0.43182200 | -0.30932400 |
|       | H  | 2.17623400  | 0.32217500  | -0.90865800 |
|       | H  | 2.37809700  | -0.98441400 | 0.30012800  |
|       | H  | 1.11623200  | -1.12353900 | -0.95849100 |
| IMa12 | O  | 0.79579600  | 0.00001400  | -0.00818400 |
|       | C  | -0.58144500 | 0.00005300  | -0.01020700 |
|       | H  | -1.00469000 | -0.90341200 | -0.46513400 |
|       | H  | -0.86825600 | -0.00203800 | 1.05377900  |
|       | H  | -1.00475300 | 0.90502000  | -0.46193000 |
| IMa13 | C  | -0.93042700 | 0.52616300  | -0.82162000 |
|       | H  | -0.80745000 | 0.04346300  | -1.79376200 |
|       | H  | -1.35909800 | 1.51854400  | -0.96858000 |
|       | C  | 0.41565700  | 0.66223800  | -0.10767900 |
|       | C  | 0.97781500  | -0.72826100 | 0.27779900  |
|       | C  | 1.21944700  | -1.66912100 | -0.84426200 |
|       | H  | 1.39454400  | 0.74783900  | -1.79699700 |
|       | H  | 1.68341800  | -2.61674000 | -0.60272600 |
|       | H  | 0.90216900  | -1.48167900 | -1.86276000 |
|       | C  | 0.32836000  | 1.55574300  | 1.11127500  |
|       | H  | -0.37944600 | 1.14841700  | 1.83353400  |
|       | H  | 1.30843200  | 1.62109100  | 1.58470000  |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | H  | 0.00837500  | 2.55251300  | 0.79612400  |
|       | O  | 1.23806600  | -1.02268100 | 1.40091400  |
|       | Cl | -2.08108900 | -0.45678400 | 0.11495400  |
|       | O  | 1.33224100  | 1.29159300  | -1.00551700 |
| IMa14 | C  | -0.49846500 | 0.72767700  | -0.44623200 |
|       | C  | 0.23988100  | 0.55825900  | 0.89156400  |
|       | C  | 1.72706900  | 0.20519500  | 0.86959200  |
|       | H  | 1.98883400  | -0.31804200 | 1.78953000  |
|       | H  | 2.31266000  | 1.12238700  | 0.76515300  |
|       | C  | -1.64542200 | 1.70745800  | -0.27830900 |
|       | H  | -2.34290300 | 1.35777700  | 0.48214400  |
|       | H  | -1.24919300 | 2.67894600  | 0.02525400  |
|       | H  | -2.15966100 | 1.81699000  | -1.23644000 |
|       | O  | -0.28223500 | 0.77642300  | 1.96557800  |
|       | O  | 2.02882100  | -0.65046800 | -0.26239500 |
|       | O  | 3.30748900  | -0.88464900 | -0.34792200 |
|       | O  | 0.38225900  | 1.29430400  | -1.41374500 |
|       | H  | 1.02539500  | 0.61618300  | -1.64893900 |
|       | C  | -0.97889400 | -0.63002700 | -0.97717900 |
|       | H  | -0.12839800 | -1.27926500 | -1.18779700 |
|       | H  | -1.54428500 | -0.45384500 | -1.89403300 |
|       | Cl | -2.02694900 | -1.48455200 | 0.17743300  |
| IMa15 | C  | 1.35325100  | -0.69602200 | -0.34294100 |
|       | C  | 0.52463500  | -0.65005600 | 0.95013900  |
|       | C  | -0.98890300 | -0.86893700 | 0.84975400  |
|       | H  | -1.46753200 | -0.36490900 | 1.69297100  |
|       | H  | -1.18102500 | -1.94655500 | 0.89731800  |
|       | C  | 2.77681900  | -1.11853700 | -0.03238900 |
|       | H  | 3.24423800  | -0.42130100 | 0.66236600  |
|       | H  | 2.76840900  | -2.11378400 | 0.41719400  |
|       | H  | 3.34563900  | -1.15456500 | -0.96515100 |
|       | O  | 1.01999400  | -0.52769200 | 2.05148700  |
|       | O  | -1.46781700 | -0.36006900 | -0.39866600 |
|       | O  | -2.82242700 | -0.76136600 | -0.53339300 |
|       | N  | -3.71884700 | 0.48666200  | -0.10369900 |
|       | O  | -3.09098700 | 1.38577300  | 0.24393500  |
|       | O  | 0.81708100  | -1.67645900 | -1.22588400 |
|       | H  | -0.07389300 | -1.38225900 | -1.45469600 |
|       | C  | 1.30049800  | 0.66192200  | -1.05814400 |
|       | H  | 0.27800700  | 0.89186600  | -1.35705300 |
|       | H  | 1.94207200  | 0.60655400  | -1.93929000 |
|       | Cl | 1.86655700  | 2.00156500  | -0.03094800 |
| IMa16 | C  | -0.00841900 | 0.79393800  | -0.24020000 |
|       | C  | 0.75858100  | 0.00951300  | 0.83466000  |
|       | C  | 1.98626300  | -0.81148500 | 0.39283300  |
|       | H  | 2.14166500  | -1.63857500 | 1.09651600  |
|       | H  | 2.84888300  | -0.12464300 | 0.49660200  |
|       | C  | -0.78027500 | 1.93392000  | 0.39575200  |
|       | H  | -1.49366700 | 1.55703300  | 1.12823300  |
|       | H  | -0.08269000 | 2.60765600  | 0.89774200  |
|       | H  | -1.30594700 | 2.48549800  | -0.38800700 |
|       | O  | 0.47955900  | 0.04106100  | 2.01369000  |
|       | O  | 2.01942300  | -1.20142400 | -0.92243100 |
|       | O  | 0.91445700  | 1.38023100  | -1.15497400 |
|       | H  | 1.34908900  | 0.64659200  | -1.60635100 |
|       | C  | -0.92457300 | -0.14702200 | -1.03401400 |
|       | H  | -0.33343600 | -0.88784000 | -1.57453000 |
|       | H  | -1.49567600 | 0.45215900  | -1.74529000 |



|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | Cl | -2.06618800 | -1.03117700 | 0.00650800  |
| IMb1 | C  | -0.90887300 | -0.81547100 | -0.40171700 |
|      | H  | -1.02657900 | -1.89850000 | -0.31499700 |
|      | H  | -0.99335700 | -0.50903100 | -1.44417300 |
|      | C  | 0.39089700  | -0.35842200 | 0.24254600  |
|      | C  | 0.53899200  | 1.17995400  | 0.18867100  |
|      | C  | 0.15567900  | 1.87592400  | -1.09827600 |
|      | H  | -0.93688400 | 1.92114400  | -1.15827500 |
|      | H  | 0.55057300  | 2.89178500  | -1.07596500 |
|      | H  | 0.52935200  | 1.34275900  | -1.97499600 |
|      | C  | 0.54062500  | -0.88034700 | 1.65853400  |
|      | H  | 1.48877800  | -0.55019000 | 2.08261200  |
|      | H  | -0.27201400 | -0.48739400 | 2.27497100  |
|      | H  | 0.50077400  | -1.97244000 | 1.65648900  |
|      | O  | 0.93588700  | 1.78082300  | 1.16547900  |
|      | Cl | 1.70638300  | -1.03409800 | -0.78437200 |
|      | O  | -1.97454900 | -0.17050300 | 0.34385600  |
|      | O  | -3.10547200 | -0.25635700 | -0.29057200 |
| IMb2 | C  | -0.33892400 | -0.81182300 | -0.34557400 |
|      | H  | -0.36867200 | -1.89797100 | -0.47176800 |
|      | H  | -0.59519300 | -0.32139200 | -1.28986500 |
|      | C  | 1.04191900  | -0.38904900 | 0.14826600  |
|      | C  | 1.11130900  | 1.13061400  | 0.42240500  |
|      | C  | 0.48761800  | 2.05505400  | -0.59799200 |
|      | H  | -0.59947500 | 2.00846400  | -0.48135700 |
|      | H  | 0.82715900  | 3.07219600  | -0.40105600 |
|      | H  | 0.74057000  | 1.76140500  | -1.61891700 |
|      | C  | 1.48275300  | -1.19153100 | 1.35689500  |
|      | H  | 2.48005500  | -0.88230500 | 1.66971600  |
|      | H  | 0.78555700  | -1.01303700 | 2.17846800  |
|      | H  | 1.49003000  | -2.25610700 | 1.11027900  |
|      | O  | 1.63834300  | 1.53632800  | 1.43816300  |
|      | Cl | 2.16812100  | -0.71173500 | -1.22076200 |
|      | O  | -1.24271800 | -0.41668500 | 0.68892300  |
|      | O  | -2.48684300 | -1.06065900 | 0.43258700  |
|      | N  | -3.42018800 | -0.12667200 | -0.28584000 |
|      | O  | -2.95688400 | 0.91043500  | -0.54038100 |
| IMb3 | C  | -0.14826700 | 1.40254400  | -0.70008800 |
|      | H  | -1.06452700 | 2.01259100  | -0.72170200 |
|      | H  | 0.03230200  | 1.10023300  | -1.74387100 |
|      | C  | -0.34237100 | 0.18642000  | 0.21088700  |
|      | C  | 0.93040500  | -0.68421400 | 0.25743800  |
|      | C  | 1.62444800  | -0.98491200 | -1.05360800 |
|      | H  | 2.21801100  | -0.10985600 | -1.33903200 |
|      | H  | 2.29654800  | -1.83077000 | -0.90690800 |
|      | H  | 0.91311100  | -1.19892100 | -1.85393800 |
|      | C  | -0.77196200 | 0.60597200  | 1.60261600  |
|      | H  | -0.89543000 | -0.26605300 | 2.24458200  |
|      | H  | 0.00435100  | 1.24543600  | 2.03249600  |
|      | H  | -1.71310400 | 1.15952600  | 1.55057400  |
|      | O  | 1.35483800  | -1.08518000 | 1.32207200  |
|      | Cl | -1.63394800 | -0.82447900 | -0.53529200 |
|      | O  | 0.92420500  | 2.17881700  | -0.33028600 |
| IMb4 | C  | 0.32958000  | 0.41652100  | -0.00002500 |
|      | C  | -1.10723300 | 0.03128000  | 0.00003300  |
|      | C  | -1.43622100 | -1.44638500 | -0.00005500 |
|      | H  | -1.00574100 | -1.93050400 | 0.88033400  |

|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | H  | -2.51995100 | -1.55179400 | 0.00012200  |
|      | H  | -1.00606400 | -1.93028000 | -0.88073000 |
|      | C  | 0.75127600  | 1.84002300  | -0.00004600 |
|      | H  | 1.35899300  | 2.06290400  | -0.88404200 |
|      | H  | -0.14126900 | 2.46583500  | -0.00012500 |
|      | H  | 1.35891600  | 2.06298300  | 0.88398100  |
|      | O  | -1.94712700 | 0.88668000  | 0.00006500  |
|      | Cl | 1.54751300  | -0.78360100 | 0.00002900  |
| IMb5 | C  | -0.36889600 | 0.17810100  | 0.19628500  |
|      | C  | 0.94119900  | -0.63501300 | 0.29524700  |
|      | C  | 1.76566000  | -0.76301600 | -0.96228200 |
|      | H  | 1.13830700  | -0.77481000 | -1.85509900 |
|      | H  | 2.43207100  | 0.10132700  | -1.02911800 |
|      | H  | 2.36471400  | -1.67159900 | -0.89630900 |
|      | C  | -0.87427100 | 0.68421200  | 1.52190100  |
|      | H  | -1.03621700 | -0.16126400 | 2.18982800  |
|      | H  | -0.12137400 | 1.34350400  | 1.95730300  |
|      | H  | -1.80792100 | 1.22941200  | 1.37263500  |
|      | O  | 1.23655600  | -1.14255900 | 1.35562100  |
|      | O  | -0.18101100 | 1.29578200  | -0.73310300 |
|      | O  | 0.80572600  | 2.03606100  | -0.32761600 |
|      | Cl | -1.56717100 | -0.84509100 | -0.61208000 |
| IMb6 | C  | -0.36275600 | 0.33928200  | 0.17943400  |
|      | C  | -1.36008500 | -0.83654400 | 0.29070400  |
|      | C  | -1.62186600 | -1.61497700 | -0.97371300 |
|      | H  | -1.69170100 | -0.95111500 | -1.83721000 |
|      | H  | -0.77828700 | -2.29011000 | -1.14270100 |
|      | H  | -2.53826600 | -2.19255500 | -0.84936100 |
|      | C  | 0.21395400  | 0.75213400  | 1.51262700  |
|      | H  | -0.59799700 | 1.01260200  | 2.19064000  |
|      | H  | 0.76214100  | -0.08758200 | 1.94443400  |
|      | H  | 0.87436000  | 1.61001000  | 1.37538600  |
|      | O  | -1.87836100 | -1.07937700 | 1.36091300  |
|      | O  | 0.63417100  | 0.04861100  | -0.80658300 |
|      | O  | 1.31885500  | -1.11416200 | -0.34265200 |
|      | N  | 2.80694600  | -0.64341300 | 0.07216100  |
|      | O  | 2.96975800  | 0.48500000  | -0.05509000 |
|      | Cl | -1.24998400 | 1.69662900  | -0.55843000 |
| IMb7 | C  | 0.36530800  | 0.27629100  | 0.36260800  |
|      | C  | -1.09312500 | 0.16640400  | -0.23140200 |
|      | C  | -1.94001300 | -0.92987500 | 0.35687200  |
|      | H  | -1.37944600 | -1.86693400 | 0.37643800  |
|      | H  | -2.17767600 | -0.65912100 | 1.39077500  |
|      | H  | -2.85740800 | -1.03586900 | -0.22192800 |
|      | C  | 0.98020900  | 1.64200400  | 0.08308400  |
|      | H  | 0.93937700  | 1.82434300  | -0.99016700 |
|      | H  | 0.39896600  | 2.40165100  | 0.60925200  |
|      | H  | 2.01483700  | 1.65637900  | 0.42795800  |
|      | O  | -1.44263000 | 0.93795500  | -1.08962900 |
|      | O  | 0.30990500  | 0.02806300  | 1.66733800  |
|      | Cl | 1.30875700  | -0.99867900 | -0.56711600 |
| IMb8 | C  | -0.43676200 | -1.38443700 | -0.55074800 |
|      | H  | 0.15653600  | -2.30389500 | -0.46535300 |
|      | H  | -0.47162300 | -1.09095200 | -1.60590200 |
|      | C  | 0.24744300  | -0.29776300 | 0.27002500  |
|      | C  | -0.50413200 | 1.05353300  | 0.20884000  |
|      | C  | -1.14758000 | 1.42781800  | -1.10654500 |
|      | H  | -2.01223700 | 0.77602100  | -1.26204900 |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | H  | -1.47641500 | 2.46561600  | -1.05024000 |
|       | H  | -0.45488400 | 1.29588600  | -1.94093700 |
|       | C  | 0.51383100  | -0.71776800 | 1.65529400  |
|       | H  | 0.57926300  | 0.02781900  | 2.43371700  |
|       | H  | -2.16321400 | -2.24821500 | -0.47473600 |
|       | H  | 0.80164200  | -1.74270200 | 1.84964400  |
|       | O  | -0.55906100 | 1.76614200  | 1.18932800  |
|       | Cl | 1.84530300  | 0.02645700  | -0.57996500 |
|       | O  | -1.73669200 | -1.53084800 | -0.00007100 |
| IMb9  | C  | 0.31200200  | 1.22804700  | -0.88614600 |
|       | H  | -0.25738500 | 2.16640000  | -0.84846500 |
|       | H  | 0.16985300  | 0.78591000  | -1.87339400 |
|       | C  | -0.22461300 | 0.28721300  | 0.19955800  |
|       | C  | 0.61417500  | -1.01247500 | 0.21847200  |
|       | C  | 0.63146100  | -1.81441100 | -1.01841400 |
|       | H  | 1.83761800  | 1.93679000  | 0.06181700  |
|       | H  | 1.25859800  | -2.69615200 | -1.01956100 |
|       | H  | 0.05274000  | -1.55454600 | -1.89323000 |
|       | C  | -0.23021600 | 0.93371600  | 1.57214900  |
|       | H  | -0.63116700 | 0.24520700  | 2.31639000  |
|       | H  | 0.79452700  | 1.17036200  | 1.86993100  |
|       | H  | -0.83691200 | 1.84292600  | 1.55230400  |
|       | O  | 1.22814100  | -1.32611500 | 1.19243100  |
|       | Cl | -1.90962300 | -0.14352000 | -0.25225200 |
|       | O  | 1.70421700  | 1.42741500  | -0.74133500 |
| IMb10 | C  | 1.25580800  | -1.04919600 | -0.98340800 |
|       | H  | 2.29583200  | -1.06612300 | -1.33244000 |
|       | H  | 0.62216000  | -0.81792500 | -1.84144400 |
|       | C  | 1.11215600  | 0.03022200  | 0.09361800  |
|       | C  | -0.32264200 | 0.05715300  | 0.64779300  |
|       | C  | -1.43854300 | -0.06509900 | -0.37476100 |
|       | H  | 1.50295900  | -2.63268100 | 0.10168700  |
|       | H  | -1.50151700 | -1.10659700 | -0.70222600 |
|       | H  | -1.28021500 | 0.59196400  | -1.23290600 |
|       | C  | 2.11528500  | -0.13609600 | 1.21950000  |
|       | H  | 1.99963700  | 0.66002000  | 1.95493900  |
|       | H  | 1.93699800  | -1.08620900 | 1.73235800  |
|       | H  | 3.13141500  | -0.11612500 | 0.81711800  |
|       | O  | -0.54297800 | 0.14498900  | 1.83549900  |
|       | Cl | 1.38791000  | 1.61804800  | -0.70799800 |
|       | O  | 0.82346500  | -2.30606000 | -0.49310200 |
|       | O  | -2.67719200 | 0.29531400  | 0.26838200  |
|       | O  | -3.68256000 | -0.00362200 | -0.49547700 |
| IMb11 | C  | 1.91971600  | -0.59955700 | -1.25544700 |
|       | H  | 2.85899500  | -0.25322000 | -1.70499400 |
|       | H  | 1.11721100  | -0.39610400 | -1.96634600 |
|       | C  | 1.68512200  | 0.16748800  | 0.04892400  |
|       | C  | 0.38878900  | -0.29651000 | 0.73873700  |
|       | C  | -0.81019000 | -0.51948200 | -0.16945700 |
|       | H  | 2.73203500  | -2.22282800 | -0.58781600 |
|       | H  | -0.63865700 | -1.44616200 | -0.72996900 |
|       | H  | -0.91840900 | 0.31788100  | -0.86736300 |
|       | C  | 2.86136000  | 0.06148400  | 1.00148700  |
|       | H  | 2.67446500  | 0.64213800  | 1.90472300  |
|       | H  | 2.99566400  | -0.98170000 | 1.30360200  |
|       | H  | 3.76874100  | 0.42721500  | 0.51362300  |
|       | O  | 0.34481600  | -0.48714600 | 1.93390500  |
|       | Cl | 1.44657200  | 1.89673700  | -0.39381300 |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | O  | 1.90843900  | -1.99743400 | -1.02711600 |
|       | O  | -1.95123400 | -0.64976500 | 0.66452600  |
|       | O  | -3.03409000 | -0.99084600 | -0.19174700 |
|       | N  | -3.81873700 | 0.26864800  | -0.52854200 |
|       | O  | -3.35785500 | 1.23858800  | -0.08660700 |
| IMb12 | C  | -0.97289800 | 1.06497500  | -0.91432000 |
|       | H  | -2.04902100 | 1.13067600  | -1.11881700 |
|       | H  | -0.47270000 | 0.80052600  | -1.84700200 |
|       | C  | -0.73334400 | -0.01305900 | 0.14711000  |
|       | C  | 0.75798200  | -0.08077000 | 0.52514400  |
|       | C  | 1.76911600  | -0.02013700 | -0.62606100 |
|       | H  | -0.97820200 | 2.64992900  | 0.19673600  |
|       | H  | 1.79741600  | 1.03328900  | -0.95898200 |
|       | H  | 1.44037400  | -0.60987000 | -1.49299800 |
|       | C  | -1.59223800 | 0.19016800  | 1.38109500  |
|       | H  | -1.40918900 | -0.60130000 | 2.10779100  |
|       | H  | -1.33000800 | 1.13951200  | 1.85857100  |
|       | H  | -2.64947500 | 0.19434200  | 1.10319900  |
|       | O  | 1.10880500  | -0.15143500 | 1.68114500  |
|       | Cl | -1.15472000 | -1.59585600 | -0.60217700 |
|       | O  | -0.42048900 | 2.30488100  | -0.50487100 |
|       | O  | 3.05035100  | -0.33527200 | -0.26243600 |
| IMc1  | C  | 1.08228000  | 0.43040300  | -0.61138200 |
|       | H  | 1.59776500  | 1.34727100  | -0.90414000 |
|       | H  | 1.16413400  | -0.33444500 | -1.38309300 |
|       | C  | -0.34396400 | 0.68467300  | -0.23116300 |
|       | C  | -1.20871800 | -0.53631700 | -0.11010300 |
|       | C  | -2.59996100 | -0.39151600 | 0.47018100  |
|       | H  | -3.20952300 | 0.26745900  | -0.15520500 |
|       | H  | -3.06035700 | -1.37841200 | 0.51439800  |
|       | H  | -2.55267100 | 0.04233500  | 1.47292200  |
|       | C  | -0.79976900 | 1.93244800  | -0.01123100 |
|       | H  | -1.82887500 | 2.12745800  | 0.27031900  |
|       | H  | -0.14314600 | 2.79102300  | -0.11714900 |
|       | O  | -0.77412100 | -1.61555300 | -0.48240800 |
|       | O  | 1.74052800  | -0.08911400 | 0.58226900  |
|       | O  | 2.94027700  | -0.49293700 | 0.30815600  |
| IMc2  | C  | 0.30380200  | 0.04430800  | -0.77243100 |
|       | H  | 0.89889300  | 0.80181600  | -1.29277900 |
|       | H  | 0.16928100  | -0.84330400 | -1.39328700 |
|       | C  | -1.02274800 | 0.59784700  | -0.34161600 |
|       | C  | -2.08626200 | -0.41792100 | -0.03618400 |
|       | C  | -3.35530500 | 0.04459500  | 0.65004000  |
|       | H  | -3.88847200 | 0.76641900  | 0.02420900  |
|       | H  | -3.99050000 | -0.82391800 | 0.82380800  |
|       | H  | -3.11978300 | 0.53077100  | 1.60083200  |
|       | C  | -1.21542000 | 1.92343700  | -0.21333000 |
|       | H  | -2.16073300 | 2.33938000  | 0.11835800  |
|       | H  | -0.41873500 | 2.62372400  | -0.44671500 |
|       | O  | -1.91281000 | -1.58582000 | -0.34644300 |
|       | O  | 0.94307600  | -0.33563600 | 0.45552200  |
|       | O  | 2.09940000  | -1.09658400 | 0.11347300  |
|       | N  | 3.29801100  | -0.22928800 | 0.09375800  |
|       | O  | 3.08028000  | 0.90010800  | 0.30124800  |
| IMc3  | C  | 1.61784000  | -0.03102300 | -0.36824900 |
|       | H  | 2.33611900  | 0.71989800  | -0.72787400 |
|       | H  | 1.57592400  | -0.83856000 | -1.11653000 |
|       | C  | 0.24107100  | 0.56590100  | -0.18897100 |

|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | C  | -0.88471000 | -0.41599100 | -0.10040200 |
|      | C  | -2.24448000 | 0.06581100  | 0.36265900  |
|      | H  | -2.64436000 | 0.81082900  | -0.33163500 |
|      | H  | -2.91958100 | -0.78898800 | 0.40508100  |
|      | H  | -2.16909100 | 0.53121300  | 1.34937100  |
|      | C  | 0.06011000  | 1.90173200  | -0.10090200 |
|      | H  | -0.91821300 | 2.34420700  | 0.05296400  |
|      | H  | 0.90327700  | 2.58125700  | -0.18822300 |
|      | O  | -0.68903800 | -1.58427900 | -0.40951600 |
|      | O  | 2.07615500  | -0.65052500 | 0.77602000  |
| IMc4 | C  | 0.86994100  | -0.50461500 | -0.28848800 |
|      | C  | -0.46814100 | 0.17588500  | -0.07262600 |
|      | C  | -1.63001400 | -0.76623400 | 0.10608500  |
|      | H  | -1.41074100 | -1.45411400 | 0.92832100  |
|      | H  | -2.54195100 | -0.20344700 | 0.30435400  |
|      | H  | -1.73629700 | -1.36742400 | -0.80231700 |
|      | C  | 2.04751100  | -0.20577400 | 0.12601300  |
|      | H  | 2.20285900  | 0.71915700  | 0.68497300  |
|      | H  | 2.91490400  | -0.83122600 | -0.06152500 |
|      | O  | -0.54306900 | 1.36768500  | -0.03496400 |
| IMc5 | C  | -1.20778800 | -0.77198900 | -0.07267000 |
|      | H  | -0.99691300 | -1.49251200 | 0.73145800  |
|      | H  | -1.10039200 | -1.30650900 | -1.02767300 |
|      | C  | -0.18727400 | 0.33565200  | -0.01910300 |
|      | C  | 1.26569100  | -0.01196700 | 0.00624700  |
|      | C  | 1.62016300  | -1.47446000 | 0.01014500  |
|      | H  | 2.36690700  | -1.81184900 | -0.69726800 |
|      | H  | 1.43884600  | -2.07152000 | 0.89663100  |
|      | H  | -3.12457200 | -0.93147600 | -0.09817000 |
|      | C  | -0.54339100 | 1.65290200  | 0.00080500  |
|      | H  | 0.23747300  | 2.40477500  | 0.03420600  |
|      | H  | -1.58495100 | 1.94654300  | -0.01076700 |
|      | O  | 2.13941200  | 0.82821500  | 0.01306900  |
|      | O  | -2.50451200 | -0.21800000 | 0.06431000  |
| Pa1  | C  | -0.68956100 | 0.34656800  | -0.00002700 |
|      | C  | 0.68955300  | -0.34655600 | -0.00026200 |
|      | C  | 1.88975400  | 0.56389500  | -0.00003400 |
|      | H  | 1.86126600  | 1.21150300  | 0.88041900  |
|      | H  | 2.79954500  | -0.03617900 | -0.00523200 |
|      | H  | 1.85610100  | 1.22036400  | -0.87357200 |
|      | C  | -1.88976100 | -0.56390500 | 0.00017800  |
|      | H  | -1.86029900 | -1.21357300 | -0.87870400 |
|      | H  | -1.85705400 | -1.21833500 | 0.87530300  |
|      | H  | -2.79956300 | 0.03616400  | 0.00310200  |
|      | O  | 0.74956900  | -1.56403900 | -0.00000400 |
|      | O  | -0.74955700 | 1.56404400  | -0.00005100 |
| Pa2  | C  | 0.67255700  | 0.42467600  | -0.00009000 |
|      | H  | 0.73354100  | 1.51938700  | 0.00020400  |
|      | O  | 1.58587900  | -0.33513100 | 0.00002700  |
|      | Cl | -1.02681900 | -0.08155300 | 0.00000700  |
| Pa3  | C  | 0.30079300  | -0.80440000 | 0.39945900  |
|      | H  | 0.32482700  | -1.80403900 | -0.03137300 |
|      | H  | 0.35381200  | -0.86972000 | 1.48956100  |
|      | C  | -1.02252400 | -0.14176300 | 0.02031400  |
|      | C  | -1.11041100 | 1.36320300  | 0.11042400  |
|      | H  | -0.60796700 | 1.81125400  | -0.75124000 |
|      | H  | -2.16055700 | 1.65489600  | 0.11306100  |
|      | H  | -0.60223900 | 1.73054300  | 1.00568000  |

|     |    |             |             |             |
|-----|----|-------------|-------------|-------------|
|     | Cl | 1.72850300  | 0.10224200  | -0.15634300 |
|     | O  | -1.96244600 | -0.84541000 | -0.29362900 |
| Pa4 | C  | -0.53185400 | 0.00003800  | -0.00019100 |
|     | H  | -1.11968300 | 0.93680500  | 0.00038600  |
|     | O  | 0.67898900  | -0.00010200 | 0.00004700  |
|     | H  | -1.12111000 | -0.93621800 | 0.00038600  |
| Pa5 | C  | -0.00442100 | 0.81844300  | -0.27058500 |
|     | C  | 0.77255700  | 0.05084800  | 0.80493300  |
|     | C  | 1.75696600  | -1.02751600 | 0.33734400  |
|     | H  | 2.20780900  | -1.60004300 | 1.16957000  |
|     | C  | -0.76734700 | 1.97347100  | 0.34514600  |
|     | H  | -1.52048100 | 1.61146700  | 1.04614200  |
|     | H  | -0.07546600 | 2.62755700  | 0.87862900  |
|     | H  | -1.24889000 | 2.53936200  | -0.45644400 |
|     | O  | 0.68856100  | 0.25687700  | 2.00101800  |
|     | O  | 2.03235300  | -1.23239200 | -0.83020500 |
|     | O  | 0.92217000  | 1.37855800  | -1.19687100 |
|     | H  | 1.40502000  | 0.63656800  | -1.58151800 |
|     | C  | -0.92642900 | -0.14129200 | -1.03209700 |
|     | H  | -0.33913100 | -0.84366400 | -1.62373900 |
|     | H  | -1.58042200 | 0.43705500  | -1.68592100 |
|     | Cl | -1.94006200 | -1.09861000 | 0.07960600  |
| Pb1 | C  | 1.04989800  | -0.75965700 | -0.85136400 |
|     | H  | 0.91464000  | -0.40443700 | -1.89188500 |
|     | C  | 0.31178100  | 0.05066300  | 0.21694400  |
|     | C  | -1.19231400 | -0.32834200 | 0.20321100  |
|     | C  | -1.88325100 | -0.38199100 | -1.14122600 |
|     | H  | -1.57733700 | -1.30278200 | -1.65146300 |
|     | H  | -2.96184200 | -0.41044100 | -0.98429400 |
|     | H  | -1.61030500 | 0.46524600  | -1.77257300 |
|     | C  | 0.92131600  | -0.13529500 | 1.58936500  |
|     | H  | 0.36816400  | 0.44938700  | 2.32425600  |
|     | H  | 0.86940100  | -1.19111700 | 1.86138100  |
|     | H  | 1.96751000  | 0.17639300  | 1.57661400  |
|     | O  | -1.75445200 | -0.60157900 | 1.24267700  |
|     | Cl | 0.41487900  | 1.77675800  | -0.28415800 |
|     | O  | 1.72098300  | -1.73084700 | -0.58429400 |
| Pb2 | C  | 0.47418500  | 0.24067800  | 0.00002200  |
|     | C  | 1.30055000  | -1.01371100 | 0.00002600  |
|     | H  | 1.05298400  | -1.60812200 | -0.88171300 |
|     | H  | 2.35701900  | -0.74565900 | -0.00020500 |
|     | H  | 1.05324100  | -1.60827100 | 0.88165600  |
|     | O  | 0.85511000  | 1.36715200  | 0.00000100  |
|     | Cl | -1.29132500 | -0.13746800 | -0.00000200 |
| Pb3 | C  | 0.26227000  | 0.54093000  | -0.00002100 |
|     | C  | -0.95921900 | -0.42047100 | -0.00000600 |
|     | C  | -2.28260100 | 0.29662000  | 0.00013400  |
|     | H  | -2.35311900 | 0.94365600  | 0.87844300  |
|     | H  | -2.35333700 | 0.94354600  | -0.87823700 |
|     | H  | -3.08701200 | -0.43811500 | 0.00027600  |
|     | O  | -0.81134200 | -1.62026200 | -0.00015000 |
|     | O  | 0.15737200  | 1.73270600  | -0.00014100 |
|     | Cl | 1.81779600  | -0.28536000 | 0.00007100  |
| Pb4 | C  | -1.04905400 | 0.82235900  | -1.07040300 |
|     | H  | -2.12323700 | 0.72431900  | -1.27541900 |
|     | H  | -0.50739000 | 0.47517000  | -1.95118100 |
|     | C  | -0.70366900 | -0.04261300 | 0.14989900  |
|     | C  | 0.77329700  | 0.12901800  | 0.51301900  |

|     |    |             |             |             |
|-----|----|-------------|-------------|-------------|
|     | C  | 1.82806400  | -0.22772700 | -0.55999700 |
|     | H  | -1.25137800 | 2.54815800  | -0.22213700 |
|     | H  | 1.45837400  | -0.51405100 | -1.56052800 |
|     | C  | -1.59587700 | 0.25726100  | 1.33932600  |
|     | H  | -1.33721900 | -0.38150100 | 2.18468400  |
|     | H  | -1.44867200 | 1.29399400  | 1.65522000  |
|     | H  | -2.64263900 | 0.09465700  | 1.06978000  |
|     | O  | 1.12861400  | 0.53541100  | 1.59840500  |
|     | Cl | -0.91594100 | -1.76456200 | -0.33167100 |
|     | O  | -0.64880700 | 2.16297300  | -0.86304800 |
|     | O  | 3.00851500  | -0.18250700 | -0.29699100 |
| Pc1 | C  | -1.49278900 | -0.60849800 | -0.00013400 |
|     | H  | -1.26917400 | -1.68689700 | -0.00022400 |
|     | C  | -0.29080900 | 0.29666300  | 0.00005000  |
|     | C  | 1.06259500  | -0.34668400 | 0.00005600  |
|     | C  | 2.28784500  | 0.54405100  | -0.00031600 |
|     | H  | 2.29290800  | 1.18762900  | 0.88413700  |
|     | H  | 3.17557600  | -0.08838600 | -0.00018900 |
|     | H  | 2.29270700  | 1.18701100  | -0.88522600 |
|     | C  | -0.48521000 | 1.62895800  | 0.00029200  |
|     | H  | 0.33314400  | 2.34026100  | 0.00043100  |
|     | H  | -1.50214600 | 2.01136200  | 0.00034300  |
|     | O  | 1.15787000  | -1.56545000 | 0.00031200  |
|     | O  | -2.63447100 | -0.18929000 | -0.00018200 |
| TS1 | C  | 0.71850700  | 0.15300900  | 1.31288900  |
|     | H  | 0.64295800  | -0.84142300 | 1.73495800  |
|     | H  | 1.44815000  | 0.82311400  | 1.75449300  |
|     | C  | -0.20029300 | 0.62633600  | 0.44347200  |
|     | C  | -1.34460300 | -0.25803900 | -0.07654300 |
|     | C  | -1.29476200 | -1.73708400 | 0.23362500  |
|     | H  | -1.41295800 | -1.88893100 | 1.31106300  |
|     | H  | -2.11468100 | -2.22356100 | -0.29316700 |
|     | H  | -0.33506800 | -2.15851700 | -0.07263500 |
|     | C  | -0.20648100 | 2.02556700  | -0.06488000 |
|     | H  | -0.18865000 | 2.01913500  | -1.15781300 |
|     | H  | -1.14274700 | 2.50833600  | 0.23177800  |
|     | H  | 0.64683300  | 2.58915900  | 0.31396900  |
|     | O  | -2.23180300 | 0.25547500  | -0.69019200 |
|     | Cl | 2.01625700  | -0.45469600 | -0.55249900 |
| TS2 | C  | 0.59153700  | 0.10054600  | 1.59859400  |
|     | H  | 0.24692400  | -0.82416000 | 2.04333300  |
|     | H  | 1.40995200  | 0.61908300  | 2.08532900  |
|     | C  | 0.07079100  | 0.57150500  | 0.43504500  |
|     | C  | -1.22815300 | -0.03659100 | -0.11441600 |
|     | C  | -1.58262000 | -1.45571400 | 0.26669700  |
|     | H  | -1.92661500 | -1.46985100 | 1.30635400  |
|     | H  | -2.39798700 | -1.78481700 | -0.37706900 |
|     | H  | -0.72288100 | -2.11928700 | 0.16941600  |
|     | C  | 0.41718100  | 1.92545200  | -0.10333100 |
|     | H  | 0.37964300  | 1.92144600  | -1.19231300 |
|     | H  | -0.33376300 | 2.63803600  | 0.25240100  |
|     | H  | 1.40856200  | 2.23234900  | 0.23242000  |
|     | O  | -1.94363800 | 0.66133200  | -0.78447000 |
|     | Cl | 1.63958000  | -0.77262600 | -0.63174400 |
| TS3 | C  | -0.24202200 | -1.23456400 | 0.01338200  |
|     | H  | -1.52636300 | -0.49586200 | -0.00619700 |
|     | H  | -0.60861500 | -2.25581600 | 0.01750100  |
|     | C  | 0.92843300  | -0.71004500 | 0.01717000  |

|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | C  | 1.23075600  | 0.80842600  | -0.00791900 |
|      | C  | 0.07289600  | 1.76784700  | 0.09226400  |
|      | H  | -0.51664600 | 1.55928700  | 0.98756800  |
|      | H  | 0.46618200  | 2.78359800  | 0.12010500  |
|      | H  | -0.58506600 | 1.64292700  | -0.77100900 |
|      | C  | 2.17605100  | -1.56541100 | 0.02803000  |
|      | H  | 2.77445100  | -1.32602300 | -0.85390500 |
|      | H  | 2.77312500  | -1.31205300 | 0.90754800  |
|      | H  | 1.93233600  | -2.62852700 | 0.03775000  |
|      | O  | 2.37088200  | 1.15718900  | -0.10397200 |
|      | Cl | -2.86312600 | -0.09544500 | -0.02736100 |
| TS4  | C  | -0.37408400 | -0.75649100 | -0.09833800 |
|      | H  | -1.84654400 | -0.43072200 | -0.06808000 |
|      | H  | -0.31082200 | -1.83052800 | -0.21298900 |
|      | C  | 0.43836800  | 0.22867300  | 0.02455400  |
|      | C  | 1.97119500  | -0.03757100 | -0.04082400 |
|      | C  | 2.44184300  | -1.46081700 | 0.15223200  |
|      | H  | 2.02258000  | -2.09746200 | -0.63170300 |
|      | H  | 3.53012700  | -1.48123700 | 0.10422100  |
|      | H  | 2.09347300  | -1.83619400 | 1.11782300  |
|      | C  | 0.08176200  | 1.68090200  | 0.17015500  |
|      | H  | 0.52337500  | 2.07033200  | 1.09139600  |
|      | H  | 0.52534200  | 2.23628600  | -0.65902700 |
|      | H  | -0.99784300 | 1.82485800  | 0.18630400  |
|      | O  | 2.70840200  | 0.88383300  | -0.22721600 |
|      | Cl | -3.20949500 | -0.20318700 | -0.02099400 |
| TS5  | C  | 0.44755200  | -1.43109800 | 0.83459300  |
|      | H  | -0.43252000 | -1.07781900 | 1.36044500  |
|      | H  | 0.68211600  | -2.48682100 | 0.93923300  |
|      | C  | 1.20199700  | -0.63564800 | 0.11952100  |
|      | C  | 0.90185200  | 0.84573000  | 0.10374200  |
|      | C  | -0.52234000 | 1.34108300  | 0.33853600  |
|      | H  | -0.76026300 | 1.56950100  | 1.37766900  |
|      | H  | -0.79737200 | 2.13410200  | -0.35448900 |
|      | H  | -1.51869600 | 0.40385500  | -0.01313200 |
|      | C  | 2.45473200  | -1.03559200 | -0.60463400 |
|      | H  | 2.39115800  | -0.74907000 | -1.65888800 |
|      | H  | 3.31377000  | -0.51047600 | -0.18063500 |
|      | H  | 2.61432000  | -2.11353300 | -0.53477400 |
|      | O  | 1.75358300  | 1.66641000  | -0.07163000 |
|      | Cl | -2.73082000 | -0.29458000 | -0.30076100 |
| TS6  | C  | 0.98925400  | 1.88323600  | -0.37980100 |
|      | H  | 1.87947200  | 1.88981500  | -0.99847700 |
|      | H  | 0.44296500  | 2.81895700  | -0.30451100 |
|      | C  | 0.58540100  | 0.80678700  | 0.25635000  |
|      | C  | 1.35500400  | -0.52008400 | 0.19293600  |
|      | C  | 2.36602600  | -0.69393100 | -0.91998500 |
|      | H  | 3.16878800  | 0.04228900  | -0.82172900 |
|      | H  | 2.78113300  | -1.69891300 | -0.85386400 |
|      | H  | 1.88409900  | -0.54400500 | -1.88968900 |
|      | C  | -0.61813900 | 0.78089900  | 1.09858200  |
|      | H  | -0.57224600 | 0.09522500  | 1.94281000  |
|      | H  | -1.07463600 | 1.74760500  | 1.30555700  |
|      | H  | -1.50559900 | 0.19891500  | 0.37720900  |
|      | O  | 1.13144600  | -1.37323200 | 1.00338600  |
|      | Cl | -2.59534300 | -0.41796900 | -0.48664000 |
| TSa1 | C  | 1.15222500  | -0.94669800 | -0.84022000 |
|      | H  | 1.28657200  | -0.44112900 | -1.79630300 |



|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | H  | 0.81696900  | -1.97109100 | -1.01093000 |
|      | C  | 0.11873300  | -0.19797200 | 0.00617600  |
|      | C  | 0.62964000  | 1.21965800  | 0.34334600  |
|      | C  | 0.92504100  | 2.12913000  | -0.82827100 |
|      | H  | 0.19289000  | 1.99696300  | -1.62576700 |
|      | H  | 0.93347700  | 3.16171400  | -0.47732100 |
|      | H  | 1.92013200  | 1.88419900  | -1.21742200 |
|      | C  | -0.28032400 | -0.95527000 | 1.25543000  |
|      | H  | 0.58712200  | -1.10556200 | 1.89935600  |
|      | H  | -1.02000100 | -0.38114400 | 1.81290800  |
|      | H  | -0.69806200 | -1.92665600 | 0.97381800  |
|      | O  | 0.80440400  | 1.55138800  | 1.49862000  |
|      | Cl | 2.72901400  | -1.00977500 | -0.02072100 |
|      | O  | -0.96237200 | -0.08873800 | -0.93403700 |
|      | O  | -1.91269100 | 0.85435800  | -0.37725300 |
|      | N  | -3.29928300 | -0.17398900 | -0.31966400 |
|      | O  | -3.35094500 | -0.74555100 | 0.66714100  |
| TSa2 | C  | -0.96513100 | 0.27195000  | -1.02274800 |
|      | H  | -0.49958900 | -0.34500400 | -1.78181700 |
|      | H  | -1.25055700 | 1.27345100  | -1.32092500 |
|      | C  | 0.65635300  | 0.84379800  | -0.00688200 |
|      | C  | 1.03458600  | -0.63207700 | 0.35700500  |
|      | C  | 1.99268900  | -1.29595500 | -0.60109500 |
|      | H  | 2.97977400  | -0.84554400 | -0.45726100 |
|      | H  | 2.03708500  | -2.36405700 | -0.38634800 |
|      | H  | 1.71685800  | -1.10756100 | -1.63964000 |
|      | C  | 0.05254100  | 1.63764500  | 1.13853800  |
|      | H  | -0.67622700 | 1.06489200  | 1.70992000  |
|      | H  | 0.88055500  | 1.89716800  | 1.80635400  |
|      | H  | -0.38093400 | 2.56052500  | 0.74923200  |
|      | O  | 0.63498500  | -1.13121100 | 1.38415500  |
|      | Cl | -2.14941300 | -0.53798500 | -0.08930100 |
| TSa3 | O  | 1.25336900  | 1.38867500  | -0.92794400 |
|      | O  | 1.89698400  | 0.82279800  | -0.48714500 |
|      | O  | 1.99331000  | -0.71477400 | -1.37386600 |
|      | O  | 0.95398500  | 0.20051600  | -3.05698100 |
|      | N  | 1.48675300  | -0.70183400 | -2.50067500 |
|      | C  | 1.06168200  | 0.52039400  | 0.54037100  |
|      | H  | 1.30240300  | -0.41997000 | 1.04386100  |
|      | H  | 1.13463200  | 1.36375100  | 1.23576100  |
| TSa4 | Cl | -0.68154500 | 0.39352400  | 0.06645100  |
|      | C  | 0.33962700  | 0.56778300  | 0.53231800  |
|      | H  | 0.60195300  | 0.85152400  | 1.56243300  |
|      | H  | -0.44997400 | -0.34892600 | 0.76653500  |
|      | O  | -0.32002800 | 1.30541800  | -0.19358500 |
|      | O  | -1.62793200 | -0.88672400 | 0.32751900  |
|      | O  | -2.02973000 | -0.08680100 | -0.45005800 |
| TSa5 | Cl | 1.74304600  | -0.38614300 | -0.17611100 |
|      | C  | -1.01117900 | 0.39048200  | -0.90571600 |
|      | H  | -0.83343500 | -0.22481000 | -1.78657600 |
|      | H  | -1.60271700 | 1.26456900  | -1.18795400 |
|      | C  | 0.33598400  | 0.89175900  | -0.35143200 |
|      | C  | 1.05634600  | -0.66680700 | 0.36366600  |
|      | C  | 1.19651500  | -1.72964900 | -0.68887100 |
|      | H  | 1.52149200  | -1.24570600 | -1.60884200 |
|      | H  | 1.91393400  | -2.47500400 | -0.34113800 |
|      | H  | 0.21998700  | -2.19654600 | -0.83661800 |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | C  | 0.22739900  | 1.81333500  | 0.85577400  |
|       | H  | -0.39086700 | 1.39554600  | 1.65170500  |
|       | H  | 1.22831500  | 2.02162200  | 1.23447800  |
|       | H  | -0.21908900 | 2.75022300  | 0.50767200  |
|       | O  | 1.39711500  | -0.62934200 | 1.48882200  |
|       | Cl | -1.97838500 | -0.55014600 | 0.26601700  |
|       | O  | 1.22345100  | 1.11282500  | -1.21326500 |
| TSa6  | C  | 0.89374000  | -0.27939700 | 0.43205000  |
|       | C  | -1.13194800 | 0.13535500  | 0.05058900  |
|       | H  | -1.53546800 | 0.31044900  | 1.03921400  |
|       | H  | -1.01890200 | 1.00186800  | -0.59154600 |
|       | H  | -1.41535100 | -0.79158200 | -0.43566400 |
|       | O  | 1.53742000  | -0.50297200 | -0.49457200 |
| TSa7  | O  | 1.39830000  | 0.86601200  | -0.63169800 |
|       | O  | 1.21464500  | -0.76933000 | -1.50090100 |
|       | O  | 1.80567500  | 0.21591500  | -3.35343500 |
|       | N  | 1.46742500  | -0.69698800 | -2.67267200 |
|       | C  | 1.05998000  | 0.51652000  | 0.67112000  |
|       | H  | 1.74401800  | -0.21928000 | 1.12089200  |
|       | H  | 1.14647400  | 1.44666900  | 1.25303600  |
|       | H  | 0.02492800  | 0.15679500  | 0.77533900  |
| TSa8  | C  | 0.35469900  | 0.54105700  | 0.53523900  |
|       | H  | 0.46964100  | 0.87499300  | 1.57980500  |
|       | H  | -0.40880300 | -0.41675200 | 0.70377200  |
|       | O  | -0.32728500 | 1.28078800  | -0.24747500 |
|       | O  | -1.61892800 | -0.87703700 | 0.35227700  |
|       | O  | -2.02340900 | -0.00225400 | -0.36682600 |
|       | H  | 1.22425000  | 0.01419100  | 0.10846700  |
| TSa9  | C  | -0.88406600 | 0.54930900  | -0.85801600 |
|       | H  | -0.57024800 | 0.14019900  | -1.81996600 |
|       | H  | -1.29375200 | 1.54963400  | -1.01011400 |
|       | C  | 0.32525300  | 0.64817000  | 0.07827800  |
|       | C  | 1.01122200  | -0.73317000 | 0.23341800  |
|       | C  | 2.10566500  | -0.78103800 | -0.81916900 |
|       | H  | 2.10491700  | 0.44789500  | -0.94556700 |
|       | H  | 3.06183700  | -1.18094500 | -0.48324000 |
|       | H  | 1.78394200  | -1.19201800 | -1.77852500 |
|       | C  | 0.00379600  | 1.24875000  | 1.43635100  |
|       | H  | -0.65943000 | 0.58051800  | 1.98934700  |
|       | H  | 0.93061000  | 1.37869200  | 1.99959000  |
|       | H  | -0.47815200 | 2.22296600  | 1.31548600  |
|       | O  | 0.78997100  | -1.55586300 | 1.08270600  |
|       | Cl | -2.17787000 | -0.48984400 | -0.21350700 |
|       | O  | 1.30663400  | 1.40439900  | -0.59052700 |
| TSa10 | C  | -0.30605400 | -0.19073000 | 0.35563000  |
|       | C  | 0.93727900  | -1.08662300 | 0.41886100  |
|       | C  | 1.26918100  | -1.94188300 | -0.84169500 |
|       | H  | 1.81913300  | -2.82317300 | -0.49300500 |
|       | H  | 1.93214300  | -1.29990900 | -1.44174400 |
|       | C  | -0.16081100 | 0.98021100  | 1.30780500  |
|       | H  | -0.01768300 | 0.63268600  | 2.33070200  |
|       | H  | 0.70365200  | 1.57888800  | 1.01245900  |
|       | H  | -1.05933200 | 1.60003600  | 1.24753700  |
|       | O  | 1.70592900  | -1.12024700 | 1.35213400  |
|       | O  | 0.09517700  | -2.25870900 | -1.52227200 |
|       | O  | 0.60915500  | -2.85468200 | -3.11682000 |
|       | N  | 0.71033500  | -4.09210200 | -3.18288800 |
|       | O  | 0.51684100  | -4.86973400 | -2.30305700 |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | O  | -0.44194200 | 0.34803400  | -0.95345100 |
|       | H  | -0.52864400 | -0.41527100 | -1.54284200 |
|       | C  | -1.55514800 | -1.03369800 | 0.64748600  |
|       | H  | -1.65502900 | -1.82323800 | -0.09873600 |
|       | H  | -2.42475000 | -0.37488200 | 0.61117800  |
|       | Cl | -1.50124500 | -1.81497100 | 2.24653200  |
| TSa11 | C  | 1.24271600  | -0.33740600 | -0.42481600 |
|       | C  | 0.50790700  | -0.82915000 | 0.83916300  |
|       | C  | -1.00970700 | -1.24229700 | 0.66028200  |
|       | H  | -1.57433100 | -0.16268200 | 0.85483200  |
|       | H  | -1.36344300 | -1.82201700 | 1.53791100  |
|       | C  | 2.70331000  | -0.08090900 | -0.11423900 |
|       | H  | 2.81097200  | 0.72260800  | 0.61542500  |
|       | H  | 3.15322600  | -0.98778900 | 0.29188800  |
|       | H  | 3.21328600  | 0.18985600  | -1.04264500 |
|       | O  | 1.01925600  | -1.00393600 | 1.89914500  |
|       | O  | -1.41870100 | -1.57142000 | -0.48016700 |
|       | O  | 1.20299300  | -1.36297000 | -1.40886300 |
|       | H  | 0.26919600  | -1.55031500 | -1.57059200 |
|       | C  | 0.54118900  | 0.90114900  | -0.98617000 |
|       | H  | -0.44717900 | 0.64390800  | -1.36789500 |
|       | H  | 1.14478300  | 1.32128400  | -1.79164400 |
|       | Cl | 0.33256100  | 2.15299500  | 0.27067600  |
|       | O  | -2.55719600 | 0.61980800  | 0.40302000  |
|       | O  | -2.84292000 | 0.14050500  | -0.65989700 |
| TSb1  | C  | -0.82273400 | -0.83181600 | -0.50229900 |
|       | H  | -0.90804400 | -1.92108100 | -0.38023000 |
|       | H  | -0.71391300 | -0.59723300 | -1.57032200 |
|       | C  | 0.43159200  | -0.35744300 | 0.25431400  |
|       | C  | 0.57012700  | 1.17929500  | 0.17558000  |
|       | C  | 0.27564300  | 1.83909200  | -1.15223000 |
|       | H  | -0.80532800 | 1.80171000  | -1.32071300 |
|       | H  | 0.60187500  | 2.87842700  | -1.10524700 |
|       | H  | 0.77565000  | 1.32293500  | -1.97512900 |
|       | C  | 0.44866400  | -0.84526400 | 1.68853700  |
|       | H  | 1.34983000  | -0.49751900 | 2.19414800  |
|       | H  | -0.42565300 | -0.44590400 | 2.20726600  |
|       | H  | 0.41575200  | -1.93761100 | 1.70785400  |
|       | O  | 0.89538200  | 1.80916500  | 1.16207400  |
|       | Cl | 1.84991400  | -1.04344000 | -0.62519800 |
|       | O  | -1.86208700 | -0.12785600 | 0.10256300  |
|       | O  | -3.36313500 | -0.74553600 | -0.69817600 |
|       | N  | -3.81535000 | 0.01072100  | -1.54360000 |
|       | O  | -3.40349700 | 1.06196000  | -1.91601900 |
| TSb2  | C  | 0.64448100  | -0.40672700 | -0.70867100 |
|       | H  | 1.56760100  | 0.39172800  | -0.58710200 |
|       | H  | 0.43311300  | -0.25421200 | -1.78560000 |
|       | C  | -0.40328100 | 0.20801100  | 0.24888000  |
|       | C  | -1.71799000 | -0.60358000 | 0.17475300  |
|       | C  | -2.23791600 | -0.96512100 | -1.19917000 |
|       | H  | -1.66601100 | -1.82246000 | -1.56984300 |
|       | H  | -3.28664500 | -1.25185300 | -1.11486000 |
|       | H  | -2.12160400 | -0.14308600 | -1.90775200 |
|       | C  | 0.11107700  | 0.29251700  | 1.66960200  |
|       | H  | -0.66940400 | 0.66613900  | 2.33227100  |
|       | H  | 0.40449800  | -0.70800000 | 1.99615600  |
|       | H  | 0.97728200  | 0.95699000  | 1.71775600  |
|       | O  | -2.26967100 | -0.95880300 | 1.19624800  |

|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | Cl | -0.78037200 | 1.85731100  | -0.36917400 |
|      | O  | 1.18436700  | -1.49395900 | -0.36524000 |
|      | O  | 2.85461700  | 0.50175100  | -0.18987600 |
|      | O  | 3.13684500  | -0.61900400 | 0.11919000  |
| TSb3 | C  | 0.21956200  | 1.64568700  | -0.78225800 |
|      | H  | -0.68769100 | 2.21947500  | -0.50828500 |
|      | H  | 0.12415000  | 1.10349500  | -1.74288200 |
|      | C  | -0.40862400 | 0.07917300  | 0.30294000  |
|      | C  | 0.81927000  | -0.84260300 | 0.25012500  |
|      | C  | 1.39348500  | -1.19989900 | -1.09736900 |
|      | H  | 2.00947400  | -0.35165200 | -1.41169600 |
|      | H  | 2.02490300  | -2.08117600 | -0.98437900 |
|      | H  | 0.61897000  | -1.37435000 | -1.84578600 |
|      | C  | -0.71989400 | 0.66180500  | 1.64467100  |
|      | H  | -0.94444300 | -0.15252900 | 2.34092200  |
|      | H  | 0.15719900  | 1.20088500  | 2.00547100  |
|      | H  | -1.57910700 | 1.33266900  | 1.58603900  |
|      | O  | 1.28683200  | -1.21411800 | 1.29556700  |
|      | Cl | -1.78306000 | -0.55100600 | -0.55276800 |
|      | O  | 1.30888900  | 1.88978000  | -0.28944200 |
| TSb4 | C  | -0.22997000 | -0.65906100 | 0.07547800  |
|      | C  | -0.11683000 | 0.85708400  | 0.35457000  |
|      | C  | -0.53476300 | 1.77274000  | -0.77015500 |
|      | H  | -0.23561100 | 1.37491400  | -1.74042400 |
|      | H  | -1.62637900 | 1.84998200  | -0.76754000 |
|      | H  | -0.10484800 | 2.76062500  | -0.60070500 |
|      | C  | -0.18592200 | -1.49818800 | 1.33349700  |
|      | H  | 0.73638700  | -1.31616900 | 1.88447700  |
|      | H  | -1.02256700 | -1.21865200 | 1.98081300  |
|      | H  | -0.26404600 | -2.55202200 | 1.06131500  |
|      | O  | 0.25942400  | 1.24948800  | 1.44144700  |
|      | O  | -1.28760900 | -0.95492700 | -0.77369600 |
|      | O  | -2.73185200 | -0.44059500 | 0.15481500  |
|      | N  | -3.44097300 | -1.37570900 | 0.55031300  |
|      | O  | -3.25084600 | -2.53991900 | 0.42297000  |
|      | Cl | 1.19128800  | -1.06732200 | -0.96411600 |
| TSb5 | C  | 0.43906500  | 0.29691800  | 0.42580200  |
|      | C  | -1.12764500 | 0.18767000  | -0.23283900 |
|      | C  | -1.92215500 | -0.96553500 | 0.30482500  |
|      | H  | -1.29620000 | -1.85535900 | 0.36187200  |
|      | H  | -2.22598500 | -0.69543200 | 1.32010700  |
|      | H  | -2.79722700 | -1.12738800 | -0.32528700 |
|      | C  | 1.03325700  | 1.64047800  | 0.04189500  |
|      | H  | 0.94168000  | 1.79831100  | -1.03211900 |
|      | H  | 0.49210000  | 2.42049800  | 0.58166600  |
|      | H  | 2.08545900  | 1.65344600  | 0.33074200  |
|      | O  | -1.45096400 | 1.01735100  | -1.02028400 |
|      | O  | 0.25911500  | 0.03377200  | 1.65152000  |
|      | Cl | 1.28234300  | -1.03295500 | -0.56029300 |
| TSb6 | C  | 0.21526100  | 0.44262500  | 0.27764500  |
|      | C  | -1.03179700 | -0.49013700 | -0.00811900 |
|      | C  | -2.31221000 | 0.12025100  | 0.49971800  |
|      | H  | -2.25132800 | 0.21042800  | 1.58796300  |
|      | H  | -2.43083900 | 1.13270500  | 0.10811800  |
|      | H  | -3.15128200 | -0.51358700 | 0.21337400  |
|      | C  | 0.35695200  | 0.95181500  | -1.66693900 |
|      | H  | 0.49164200  | -0.01727600 | -2.13204100 |
|      | H  | -0.58877300 | 1.45986800  | -1.82290100 |

|       |    |             |             |             |
|-------|----|-------------|-------------|-------------|
|       | H  | 1.22980800  | 1.58613100  | -1.57423200 |
|       | O  | -0.92266500 | -1.56052900 | -0.54840100 |
|       | O  | 0.12339700  | 1.48469100  | 0.84233700  |
|       | Cl | 1.74856900  | -0.55287500 | 0.39143500  |
| TSb7  | C  | 1.12275800  | -0.43678400 | -1.04647500 |
|       | H  | 1.96931700  | 0.21636800  | -1.29562700 |
|       | H  | 0.54034700  | -0.64012800 | -1.94952900 |
|       | C  | 0.31890900  | 0.17796200  | 0.09857700  |
|       | C  | -1.06899800 | -0.47749800 | 0.26350000  |
|       | C  | -1.91978500 | -0.60923800 | -0.97905300 |
|       | H  | -1.61226900 | -1.51885200 | -1.50592800 |
|       | H  | -2.96386200 | -0.71437500 | -0.68289500 |
|       | H  | -1.79627100 | 0.24064800  | -1.65276700 |
|       | C  | 1.21738500  | -0.16069400 | 1.26979000  |
|       | H  | 0.72327200  | -0.34214500 | 2.22104600  |
|       | H  | 1.58292000  | -1.23409200 | 0.74827600  |
|       | H  | 2.12130400  | 0.44648300  | 1.32291500  |
|       | O  | -1.43455300 | -0.87342700 | 1.35116300  |
|       | Cl | 0.03500600  | 1.93355100  | -0.10887900 |
|       | O  | 1.53686900  | -1.66242000 | -0.47523600 |
| TSb8  | C  | -0.10823100 | 1.00035900  | 1.21930900  |
|       | H  | 0.35272700  | 0.60324500  | 2.13778400  |
|       | H  | -1.03937100 | 1.51743800  | 1.48352500  |
|       | C  | -0.43677500 | -0.19743900 | 0.32157500  |
|       | C  | 0.90180900  | -0.79469900 | -0.15109100 |
|       | C  | 1.89034600  | 0.23807400  | -0.63250000 |
|       | H  | 1.53678600  | 1.26535300  | -0.05420300 |
|       | H  | 2.91661100  | 0.00187100  | -0.35256100 |
|       | H  | 1.77587100  | 0.47564000  | -1.69065300 |
|       | C  | -1.30757400 | -1.22205600 | 1.01588400  |
|       | H  | -1.48113400 | -2.07258500 | 0.35547100  |
|       | H  | -0.80201600 | -1.58559600 | 1.91515500  |
|       | H  | -2.26628100 | -0.77624100 | 1.29199000  |
|       | O  | 1.13972300  | -1.97727800 | -0.08256300 |
|       | Cl | -1.25800900 | 0.39062200  | -1.16457900 |
|       | O  | 0.70471500  | 1.95038600  | 0.59159700  |
| TSb9  | C  | -0.12941900 | 1.07549400  | -0.88343400 |
|       | H  | -1.05965900 | 1.65737100  | -0.83357700 |
|       | H  | -0.08958700 | 0.58769600  | -1.85909200 |
|       | C  | -0.17070500 | 0.01490300  | 0.23004200  |
|       | C  | 1.13822500  | -0.78572100 | 0.19777700  |
|       | C  | 1.34122600  | -1.79396500 | -0.95732600 |
|       | H  | 0.93186600  | 2.43393000  | -0.01502400 |
|       | H  | 2.40758200  | -1.76242500 | -1.21847000 |
|       | H  | 0.72542200  | -1.50203500 | -1.81973600 |
|       | C  | -0.38170700 | 0.63714100  | 1.59995200  |
|       | H  | -0.44095200 | -0.13868300 | 2.36515300  |
|       | H  | 0.46650800  | 1.28018500  | 1.84791800  |
|       | H  | -1.30870300 | 1.21655000  | 1.60567200  |
|       | O  | 1.99423400  | -0.61901800 | 1.03859600  |
|       | Cl | -1.54788100 | -1.06800900 | -0.14339500 |
|       | O  | 1.02628100  | 1.88301400  | -0.79583900 |
|       | O  | 0.94635800  | -2.99464400 | -0.38854000 |
|       | O  | 1.19146300  | -4.23774800 | -1.69541800 |
|       | N  | 0.13994700  | -4.61587500 | -2.19498200 |
|       | O  | -0.97228100 | -4.27123900 | -1.95039700 |
| TSb10 | C  | 1.95317400  | -0.62877000 | -0.96031900 |
|       | H  | 2.96118600  | -0.24376600 | -1.16484000 |

|      |    |             |             |             |
|------|----|-------------|-------------|-------------|
|      | H  | 1.36869900  | -0.55007600 | -1.87733700 |
|      | C  | 1.32370900  | 0.21949900  | 0.15182400  |
|      | C  | -0.05709000 | -0.33885200 | 0.52651600  |
|      | C  | -1.11602400 | -0.40288000 | -0.61817200 |
|      | H  | 2.59839500  | -2.11663300 | 0.09170200  |
|      | H  | -0.79155000 | -0.11932700 | -1.63313500 |
|      | H  | -1.77380400 | 0.60244100  | -0.30491300 |
|      | C  | 2.21275700  | 0.32315300  | 1.37633200  |
|      | H  | 1.74173100  | 0.94072500  | 2.14186800  |
|      | H  | 2.35959100  | -0.67233300 | 1.80461500  |
|      | H  | 3.17714100  | 0.75803400  | 1.10055900  |
|      | O  | -0.32011900 | -0.70992500 | 1.63174700  |
|      | Cl | 1.03239800  | 1.86779500  | -0.51190400 |
|      | O  | 1.94849300  | -1.99716400 | -0.60524800 |
|      | O  | -1.95703500 | -1.34416400 | -0.51058300 |
|      | O  | -2.97458700 | 0.95936400  | 0.09641900  |
|      | O  | -3.58316600 | -0.08117200 | 0.09850900  |
| TSc1 | C  | 1.15318000  | -0.97133600 | 1.40939500  |
|      | H  | 0.82999100  | -2.01893400 | 1.51965000  |
|      | H  | 0.86646400  | -0.39781900 | 2.30110600  |
|      | C  | 0.48918900  | -0.33914900 | 0.21068400  |
|      | C  | 0.47277000  | 1.16347100  | 0.19995700  |
|      | C  | 0.19624500  | 1.87232300  | -1.11060300 |
|      | H  | -0.80619500 | 1.62805200  | -1.47463700 |
|      | H  | 0.26961400  | 2.94763700  | -0.94677800 |
|      | H  | 0.91631600  | 1.55776100  | -1.87092200 |
|      | C  | -0.00468500 | -1.08405800 | -0.79552600 |
|      | H  | -0.45797500 | -0.63955700 | -1.67562500 |
|      | H  | 0.02995200  | -2.16855600 | -0.74702100 |
|      | O  | 0.67459900  | 1.78360700  | 1.23240700  |
|      | O  | 2.51398000  | -0.85060000 | 1.12246600  |
|      | O  | 3.38513600  | -0.91503800 | 2.75488200  |
|      | N  | 3.71775000  | -2.03391900 | 3.06575700  |
|      | O  | 3.55839500  | -3.07407400 | 2.51491100  |
| TSc2 | C  | -0.75456400 | 0.66561000  | 0.70718500  |
|      | H  | -0.77682200 | 0.66210900  | 1.81541000  |
|      | H  | -1.05823700 | -0.49646200 | 0.50073700  |
|      | C  | 0.66616100  | 0.73855800  | 0.12333200  |
|      | C  | 1.45503300  | -0.56195700 | 0.12046000  |
|      | C  | 2.86461700  | -0.55200100 | -0.43523700 |
|      | H  | 3.49287000  | 0.13252100  | 0.14124500  |
|      | H  | 3.26514300  | -1.56338700 | -0.37282000 |
|      | H  | 2.85987200  | -0.21454700 | -1.47508700 |
|      | C  | 1.16706100  | 1.86421100  | -0.26932700 |
|      | H  | 2.17875600  | 1.94850500  | -0.65585000 |
|      | H  | 0.57945100  | 2.77796200  | -0.23579400 |
|      | O  | 0.95101000  | -1.56775300 | 0.55671800  |
|      | O  | -1.67786000 | 1.29531300  | 0.13023800  |
|      | O  | -2.69210800 | -0.47898300 | -0.66346200 |
|      | O  | -1.94740100 | -1.27023100 | -0.17303300 |
| TSc3 | C  | 1.65947000  | -0.22739200 | 0.38262500  |
|      | H  | 2.41781400  | 0.42810600  | -0.08918900 |
|      | H  | 1.39415900  | -1.11273100 | -0.23448800 |
|      | C  | 0.11503700  | 0.83783100  | -0.56672000 |
|      | C  | -1.10657900 | -0.04790500 | -0.68364500 |
|      | C  | -1.65127500 | -0.54239700 | 0.62967000  |
|      | H  | -2.00289600 | 0.32516100  | 1.19755400  |
|      | H  | -2.47341100 | -1.23320200 | 0.44290100  |

|      |   |             |             |             |
|------|---|-------------|-------------|-------------|
|      | H | -0.85727000 | -0.99987100 | 1.22425100  |
|      | C | 0.37204100  | 2.05076800  | -0.88827500 |
|      | H | -0.36750500 | 2.62374000  | -1.44998200 |
|      | H | 1.30425600  | 2.54560900  | -0.63371600 |
|      | O | -1.57290900 | -0.27369200 | -1.76083100 |
|      | O | 1.36472100  | -0.14008000 | 1.55004900  |
| TSc4 | C | 1.55624000  | -0.12643200 | -0.19221800 |
|      | H | 2.38640300  | 0.57959200  | -0.07097800 |
|      | H | 1.67141000  | -0.62644100 | -1.16595700 |
|      | C | 0.23406100  | 0.60348000  | -0.13845600 |
|      | C | -0.95489800 | -0.25329200 | 0.19378400  |
|      | C | -0.61028800 | -1.70078000 | 0.46768800  |
|      | H | -1.18601800 | -2.13296400 | 1.28537900  |
|      | H | -0.63333100 | -2.31705600 | -0.43504500 |
|      | H | 0.57237700  | -1.65854400 | 0.80754100  |
|      | C | 0.07014900  | 1.92091300  | -0.36878200 |
|      | H | -0.92691800 | 2.34851900  | -0.32752300 |
|      | H | 0.90955800  | 2.57128500  | -0.59482000 |
|      | O | -2.09468600 | 0.17469600  | 0.25103400  |
|      | O | 1.66860500  | -1.04766500 | 0.86991200  |