

External electric field, a potential catalyst for C-N cross-coupling reaction.

Priyanka Yadav and Pradeep Kumar*

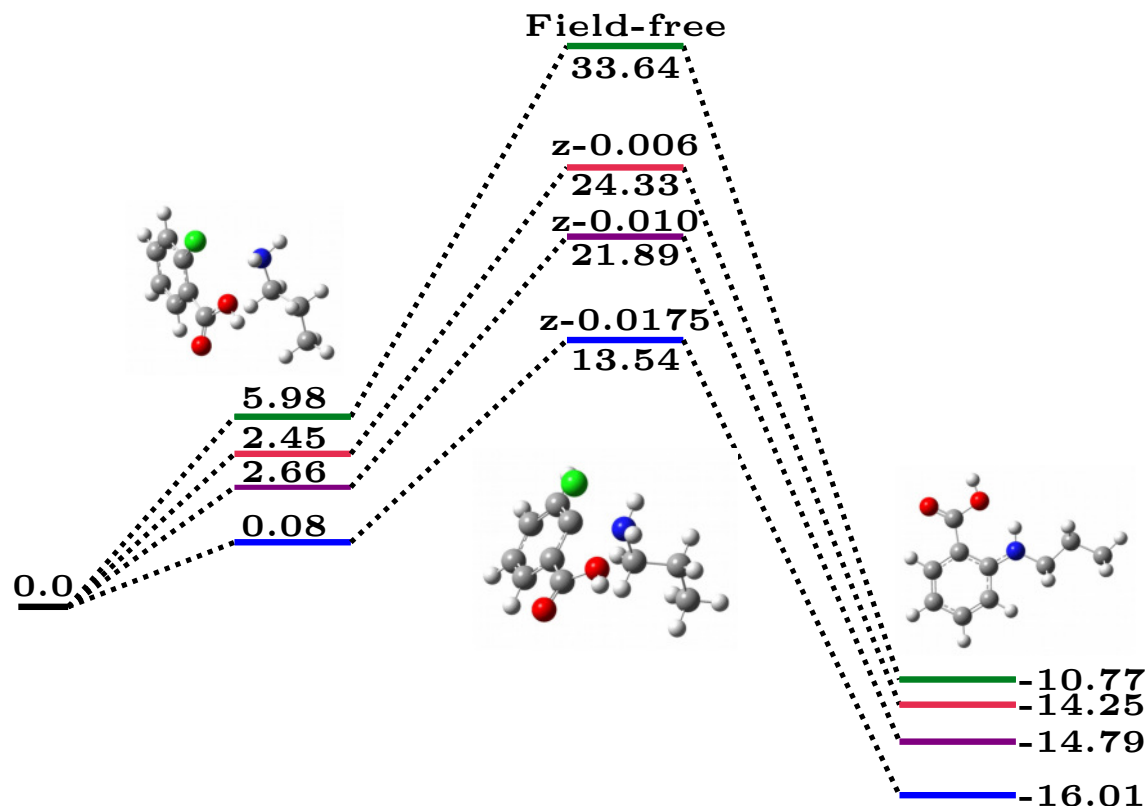
*Department of Chemistry, Malaviya National Institute of Technology Jaipur, Jaipur,
302017, India*

E-mail: pradeep.chy@mnit.ac.in

S. No.**Contents**

1. **Figure S1:** Gibbs free energy (kcal mol^{-1}) for the reaction of 2-chlorobenzoic acid and propylamine at 298 K, in the presence and absence of an EEF (a.u.) with different strengths.
2. A detailed discussion on the kinetics of the title reaction.
3. **Table S1:** Optimized geometries in Cartesian coordinates and normal mode frequencies of all species calculate at M06-2X/6-311++G** level of theory

Figure S1: Gibbs free energy (kcal mol⁻¹) for the reaction of 2-chlorobenzoic acid and propylamine at 298 K, in the presence and absence of an EEF (a.u.) with different strengths.



13. A detailed discussion on kinetics of the title reaction

Gibbs free energy profile often helps in selecting a method for the calculation of the rate of a reaction. Gibbs free energy (kcal mol⁻¹) for the reaction of 2-chlorobenzoic acid and propylamine at 298 K, in the presence and absence of an EEF (a.u.) with different strengths is shown in figure S1. It can be clearly seen from figure S1 that the Gibbs free energy barrier for the formation of reactants from RC (bimolecular dissociation) is very low and the same for RC to product is very high i.e., rate of $k_{-1} \gg \gg \gg k_{uni}$. It suggests that the time scale associated with bimolecular dissociation is much lower than the same for the unimolecular transformation. It also suggests that these reactions can occur in two steps; first, equilibration process between reactants and RC followed by a slow unimolecular transformation. Therefore, we have applied pre-equilibrium approximation.

Pre-equilibrium approximation

The reaction mechanism for the reactions can be represented as:



Here, above equation suggests that the reaction proceeds via two steps; first, a reactant-complex (RC) is formed with barrierless association process of the reactants and in second step, RC dissociates to form product through a corresponding transition state. In the first step, k_{eq} has been obtained using following formula:

$$k_{eq} = \sigma \frac{Q_{RC}}{Q_{ClC_7H_5O_2} Q_{NC_3H_9}} \exp\left[-\frac{(E_{RC} - E_R)}{RT}\right] \quad (1)$$

where σ is the symmetry number, variable Q denote the overall partition functions for the subscripted species 2-chlorobenzoic acid, propylamine and RC. E_{RC} and E_R represent energies of reactant-complex and isolated reactants respectively. All other information are given in main manuscript.

Table S1: Optimized geometries in Cartesian coordinates and normal mode frequencies of all species calculate at M06-2X/6-311++G level of theory**

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|----------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| Propylamine | C | -0.589713 | -0.506599 | -0.000062 | 128.5853 | 227.8813 | 269.1544 |
| | H | -0.482909 | -1.155335 | 0.875213 | 274.8809 | 451.3745 | 743.0273 |
| | H | -0.482880 | -1.155222 | -0.875416 | 837.8747 | 859.6549 | 914.9056 |
| | C | 0.534428 | 0.530933 | 0.000022 | 1032.626 | 1051.8929 | 1115.114 |
| | H | 0.423131 | 1.176240 | 0.878429 | 1145.9829 | 1240.2369 | 1325.4831 |
| | H | 0.423183 | 1.176348 | -0.878312 | 1326.0687 | 1387.528 | 1404.7411 |
| | C | 1.916709 | -0.117620 | 0.000016 | 1413.1898 | 1487.612 | 1498.9785 |
| | H | 2.050490 | -0.748792 | 0.882417 | 1506.0683 | 1512.5116 | 1664.8259 |
| | H | 2.050456 | -0.748866 | -0.882337 | 3042.7748 | 3055.2866 | 3059.3558 |
| | H | 2.711799 | 0.629817 | -0.000032 | 3073.0608 | 3100.0982 | 3126.9071 |
| | N | -1.950166 | 0.024287 | -0.000041 | 3138.0404 | 3533.6815 | 3616.9544 |
| | H | -2.105180 | 0.608182 | -0.814957 | | | |
| | H | -2.105470 | 0.607335 | 0.815424 | | | |
| 2-chlorobenzoic acid | C | 2.150897 | -1.464878 | 0.072839 | 37.0776 | 117.4089 | 205.094 |
| | C | 0.777854 | -1.638894 | 0.030046 | 210.5656 | 299.0164 | 346.7358 |
| | C | 2.676183 | -0.176732 | 0.071477 | 423.6018 | 464.2502 | 492.3379 |
| | H | 0.340901 | -2.629690 | 0.019544 | 545.2568 | 589.0806 | 642.5285 |
| | H | 3.747894 | -0.021313 | 0.102388 | 704.7096 | 718.0695 | 773.9525 |
| | C | -0.095189 | -0.546366 | 0.002145 | 803.2117 | 822.5303 | 905.5595 |
| | C | 1.830017 | 0.921312 | 0.018413 | 999.8686 | 1025.0865 | 1069.9436 |
| | H | 2.227195 | 1.927764 | -0.004258 | 1076.3598 | 1155.6308 | 1167.5278 |
| | C | 0.449930 | 0.742267 | -0.014365 | 1186.3 | 1232.9309 | 1292.1674 |
| | Cl | -0.517117 | 2.182072 | -0.140337 | 1317.9457 | 1402.4115 | 1481.9338 |
| | H | 2.806312 | -2.325859 | 0.104206 | 1521.3203 | 1641.1558 | 1670.3679 |
| | C | -1.549287 | -0.900180 | -0.013691 | 1848.1569 | 3211.6582 | 3223.2439 |
| | O | -1.960449 | -1.958617 | -0.408359 | 3232.2715 | 3237.1938 | 3830.7425 |
| | O | -2.354161 | 0.038478 | 0.498143 | | | |
| | H | -3.25686 | -0.304204 | 0.444392 | | | |
| RC | C | -2.085884 | 2.299789 | 0.329199 | 15.6827 | 23.7315 | 34.0912 |
| | C | -1.136963 | 1.793431 | -0.541871 | 40.0739 | 62.8699 | 105.0243 |
| | C | -2.861659 | 1.421573 | 1.078934 | 116.1612 | 125.3309 | 190.8297 |
| | H | -0.522130 | 2.452649 | -1.142282 | 208.9384 | 216.8357 | 239.3952 |
| | H | -3.608613 | 1.800052 | 1.766355 | 275.7751 | 298.1711 | 317.1265 |
| | C | -0.930385 | 0.416106 | -0.673683 | 348.2118 | 424.2071 | 455.7437 |
| | C | -2.690301 | 0.051851 | 0.946934 | 463.3084 | 485.4559 | 544.4757 |
| | H | -3.296255 | -0.641356 | 1.515217 | 595.8987 | 641.5903 | 701.0611 |
| | C | -1.727526 | -0.451179 | 0.079503 | 713.8347 | 743.703 | 768.7542 |
| | Cl | -1.624139 | -2.184860 | -0.042012 | 802.0333 | 817.2167 | 854.7126 |
| | C | 2.070788 | 0.320024 | 1.266931 | 861.4499 | 899.6375 | 922.3299 |
| | H | 1.605330 | 0.896387 | 0.459181 | 996.4092 | 1024.1389 | 1037.0081 |
| | H | 2.283092 | 1.042955 | 2.061352 | 1052.1058 | 1065.8569 | 1076.2487 |
| | C | 3.383682 | -0.279193 | 0.760558 | 1115.6462 | 1148.0917 | 1151.9313 |
| | H | 3.15254 | -1.047504 | 0.014428 | 1165.289 | 1184.5951 | 1231.1252 |
| | H | 3.886058 | -0.792313 | 1.58797 | 1240.2961 | 1291.6442 | 1319.6861 |
| | C | 4.30434 | 0.779246 | 0.158167 | 1320.7639 | 1322.344 | 1384.4927 |
| | H | 3.82477 | 1.271428 | -0.692458 | 1395.098 | 1402.1191 | 1413.7298 |
| | H | 4.545367 | 1.550583 | 0.894471 | 1481.2524 | 1490.3691 | 1500.9146 |
| | H | 5.24359 | 0.346148 | -0.190339 | 1505.7597 | 1513.6995 | 1520.8164 |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|----------|---------------------------|-----------|-----------|------------------------------|-----------|-----------|-----------|
| | N | 1.086475 | -0.631572 | 1.77182 | 1642.6843 | 1660.1626 | 1671.6546 |
| | H | 1.448779 | -1.119025 | 2.584489 | 1846.8326 | 3043.5486 | 3052.3147 |
| | H | 0.8885 | -1.335658 | 1.066277 | 3056.1457 | 3070.9633 | 3094.6966 |
| | H | -2.219808 | 3.369852 | 0.42366 | 3123.8501 | 3135.3447 | 3212.208 |
| | C | 0.167566 | 0.034005 | -1.611959 | 3222.9339 | 3233.4681 | 3239.2631 |
| | O | 0.560503 | 0.747105 | -2.496186 | 3529.3794 | 3611.6919 | 3822.9855 |
| | O | 0.736681 | -1.155121 | -1.351698 | | | |
| | H | 1.434392 | -1.280371 | -2.01006 | | | |
| TS | C | -1.225158 | 2.294814 | -1.376384 | -351.8317 | 41.27 | 53.6733 |
| | C | -1.336597 | 0.947059 | -1.627413 | 68.9531 | 84.4306 | 116.7188 |
| | C | -0.870615 | 2.689927 | -0.072574 | 152.2791 | 163.0214 | 198.9572 |
| | H | -1.630872 | 0.582150 | -2.605192 | 227.5915 | 237.8051 | 269.8517 |
| | H | -0.814167 | 3.745043 | 0.174224 | 304.8915 | 309.0103 | 366.1075 |
| | C | -1.080652 | -0.029545 | -0.649593 | 405.938 | 450.0037 | 454.2365 |
| | C | -0.627785 | 1.778345 | 0.922266 | 522.0929 | 539.0853 | 575.7164 |
| | H | -0.425091 | 2.104963 | 1.935690 | 628.7456 | 643.5728 | 715.1245 |
| | C | -0.690552 | 0.364178 | 0.673306 | 727.8389 | 747.4232 | 757.9571 |
| | Cl | -1.498845 | -0.538655 | 2.096481 | 782.258 | 817.1731 | 842.7191 |
| | C | 1.919778 | 0.093895 | 0.011500 | 891.5205 | 913.9627 | 963.181 |
| | H | 1.593436 | -0.353715 | -0.930258 | 997.2356 | 1002.5975 | 1048.6901 |
| | H | 1.830239 | 1.179537 | -0.094288 | 1053.8312 | 1064.3184 | 1095.9692 |
| | C | 3.351076 | -0.313512 | 0.339746 | 1101.4456 | 1119.5991 | 1123.654 |
| | H | 3.39891 | -1.399394 | 0.468775 | 1179.9797 | 1186.7298 | 1211.3355 |
| | H | 3.647477 | 0.134216 | 1.294056 | 1236.818 | 1276.3014 | 1324.1309 |
| | C | 4.314429 | 0.124532 | -0.761122 | 1327.3216 | 1340.9951 | 1381.8759 |
| | H | 4.048039 | -0.333148 | -1.716473 | 1389.6997 | 1415.3594 | 1420.5648 |
| | H | 4.291034 | 1.208919 | -0.890981 | 1448.9087 | 1493.5552 | 1497.364 |
| | H | 5.339007 | -0.164067 | -0.523796 | 1502.2539 | 1506.4432 | 1516.1296 |
| | N | 0.948574 | -0.315089 | 1.033077 | 1581.8319 | 1626.9534 | 1665.9838 |
| | H | 1.190292 | 0.024719 | 1.962923 | 1828.4883 | 3053.072 | 3066.0553 |
| | H | 0.819033 | -1.326794 | 1.066811 | 3075.3472 | 3089.8016 | 3128.8747 |
| | H | -1.428615 | 3.027187 | -2.144811 | 3138.7766 | 3147.6279 | 3192.5565 |
| | C | -1.173166 | -1.423978 | -1.077581 | 3210.9888 | 3213.2078 | 3244.3436 |
| | O | -1.683169 | -1.831274 | -2.090997 | 3477.2406 | 3572.7055 | 3842.1449 |
| | O | -0.54208 | -2.298695 | -0.230513 | | | |
| | H | -0.700926 | -3.1814 | -0.589228 | | | |
| PC | C | -2.952130 | 1.922903 | 0.101559 | 19.6877 | 37.3162 | 45.2878 |
| | C | -2.933982 | 0.555564 | -0.103591 | 58.5833 | 95.4333 | 96.182 |
| | C | -1.742628 | 2.609039 | 0.140415 | 116.1738 | 161.3108 | 186.723 |
| | H | -3.853774 | -0.015027 | -0.134337 | 232.7498 | 242.4643 | 280.8436 |
| | H | -1.728376 | 3.679892 | 0.306259 | 302.7414 | 315.4539 | 399.9684 |
| | C | -1.736342 | -0.145649 | -0.278042 | 428.3846 | 445.597 | 527.5395 |
| | C | -0.541841 | 1.938105 | -0.027859 | 562.2525 | 582.6316 | 602.636 |
| | H | 0.383838 | 2.494335 | 0.018987 | 647.9911 | 677.9175 | 723.2968 |
| | C | -0.507891 | 0.553949 | -0.244069 | 768.2394 | 777.5069 | 781.5799 |
| | Cl | 1.544718 | -0.608537 | 2.506283 | 814.9306 | 830.8096 | 869.9193 |
| | C | 1.935367 | 0.670411 | -0.692871 | 891.1487 | 898.2473 | 923.4745 |
| | H | 1.741163 | 1.318889 | -1.556228 | 933.908 | 998.735 | 1021.0699 |
| | H | 2.208948 | 1.307242 | 0.154747 | 1065.1161 | 1079.7376 | 1098.9036 |
| | C | 3.083103 | -0.286047 | -0.985883 | 1118.353 | 1141.4326 | 1170.0911 |
| | H | 2.812461 | -0.924542 | -1.833958 | 1182.7605 | 1191.2289 | 1227.6953 |
| | H | 3.226452 | -0.938781 | -0.119489 | 1278.6619 | 1284.6343 | 1307.5106 |
| | C | 4.373449 | 0.467886 | -1.292984 | 1330.1523 | 1338.3737 | 1345.5426 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|-------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | H | 4.250175 | 1.124484 | -2.157799 | 1379.2762 | 1415.0951 | 1421.3769 |
| | H | 4.675026 | 1.082521 | -0.441806 | 1484.2138 | 1497.36 | 1507.1173 |
| | H | 5.188212 | -0.223583 | -1.510637 | 1509.7532 | 1510.858 | 1526.3374 |
| | N | 0.73499 | -0.09274 | -0.335764 | 1557.24 | 1652.7338 | 1680.0146 |
| | H | 1.107622 | -0.479991 | 1.231911 | 1850.659 | 1989.6609 | 3033.8677 |
| | H | 0.6824 | -0.989069 | -0.804682 | 3051.8802 | 3063.9757 | 3081.1099 |
| | H | -3.890569 | 2.445363 | 0.232961 | 3102.0994 | 3134.5939 | 3146.7364 |
| | C | -1.903133 | -1.609696 | -0.48356 | 3210.0946 | 3226.1529 | 3238.0187 |
| | O | -2.949754 | -2.193449 | -0.415067 | 3247.3023 | 3594.6519 | 3831.2333 |
| | O | -0.75801 | -2.273848 | -0.780822 | | | |
| | H | -0.990441 | -3.207844 | -0.873978 | | | |
| 2-chlorobenzoic acid (-0.006) | C | 0.000000 | 0.000000 | 0.000000 | -2.7020 | 115.997 | 214.0671 |
| | Cl | 0.000000 | 0.000000 | 1.728747 | 218.7673 | 302.2931 | 350.7335 |
| | C | 0.250927 | 0.000000 | -2.784386 | 432.0412 | 470.9915 | 505.5561 |
| | C | -0.972365 | 0.245650 | -2.187668 | 534.9753 | 612.326 | 642.7302 |
| | C | 1.361351 | -0.250521 | -1.982341 | 708.0107 | 715.0047 | 765.699 |
| | H | -1.854880 | 0.447739 | -2.781387 | 806.1022 | 822.1633 | 899.8233 |
| | H | 2.330951 | -0.445677 | -2.425364 | 997.1159 | 1010.8883 | 1076.9122 |
| | C | -1.127888 | 0.247089 | -0.795919 | 1078.8016 | 1156.0754 | 1167.7591 |
| | C | 1.235132 | -0.247015 | -0.603731 | 1181.8471 | 1225.071 | 1287.1641 |
| | H | 2.090942 | -0.432513 | 0.032384 | 1320.697 | 1410.8974 | 1480.2947 |
| | H | 0.340151 | 0.003416 | -3.863960 | 1518.5824 | 1636.8366 | 1671.323 |
| | C | -2.526501 | 0.526819 | -0.327070 | 1831.212 | 3201.8088 | 3216.959 |
| | O | -3.405595 | 0.858508 | -1.082769 | 3230.6536 | 3234.0512 | 3822.1905 |
| | O | -2.7181 | 0.361621 | 0.97689 | | | |
| | H | -3.641581 | 0.570982 | 1.176699 | | | |
| Propylamine (-0.006) | N | 0.0000 | 0.000000 | 0.000000 | 129.7896 | 229.3665 | 271.8224 |
| | C | 0.0000 | 0.000000 | 2.536023 | 291.8155 | 452.2606 | 747.1028 |
| | C | 0.798202 | 0.000000 | 1.232954 | 864.4842 | 869.9635 | 945.2552 |
| | H | 1.454094 | -0.875703 | 1.206928 | 1037.4796 | 1052.1049 | 1105.9675 |
| | H | 1.453997 | 0.875780 | 1.206903 | 1148.385 | 1241.4372 | 1326.1855 |
| | H | -0.654889 | -0.878453 | 2.553747 | 1326.3786 | 1389.6495 | 1403.116 |
| | H | -0.654455 | 0.878773 | 2.553945 | 1419.9273 | 1488.2743 | 1499.7502 |
| | C | 0.904553 | -0.000344 | 3.765894 | 1505.853 | 1513.0139 | 1663.2162 |
| | H | 1.548126 | -0.883394 | 3.778341 | 3041.1719 | 3058.2374 | 3064.2859 |
| | H | 1.548523 | 0.882415 | 3.778527 | 3072.6381 | 3102.8847 | 3131.2627 |
| | H | 0.324335 | -0.000307 | 4.688902 | 3151.1958 | 3514.7424 | 3592.2543 |
| | H | -0.613535 | 0.809739 | 0.002864 | | | |
| | H | -0.613373 | -0.809863 | 0.002704 | | | |
| RC (-0.006) | C | 0.000000 | 0.000000 | 0.000000 | 19.3811 | 24.1739 | 32.5378 |
| | N | 0.000000 | 0.000000 | 3.290688 | 45.0794 | 56.2134 | 68.5358 |
| | C | 2.591700 | 0.000000 | 0.992954 | 97.8324 | 132.3002 | 137.397 |
| | C | 1.924045 | -1.197455 | 0.789817 | 179.6414 | 203.9943 | 231.2447 |
| | C | 1.958596 | 1.199680 | 0.688171 | 273.3046 | 283.989 | 292.8539 |
| | H | 2.393626 | -2.144451 | 1.028591 | 347.6449 | 404.3221 | 454.9134 |
| | H | 2.465414 | 2.141994 | 0.858706 | 455.7295 | 473.6225 | 562.7287 |
| | C | 0.612563 | -1.210552 | 0.314899 | 596.2791 | 639.4011 | 700.4756 |
| | C | 0.669832 | 1.202112 | 0.172549 | 729.584 | 750.0002 | 768.4256 |
| | H | 0.167933 | 2.129101 | -0.072463 | 799.7525 | 814.1473 | 866.2352 |
| | Cl | -1.610205 | 0.055563 | -0.675957 | 867.4679 | 895.5089 | 940.5263 |
| | C | 0.581474 | -1.211512 | 3.875242 | 985.1427 | 1019.3756 | 1038.2166 |
| | H | 0.342669 | -2.050648 | 3.210347 | 1053.0983 | 1061.4757 | 1073.5622 |
| | H | 1.671852 | -1.103369 | 3.852686 | 1111.5716 | 1148.296 | 1154.7714 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|-------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | C | 0.133565 | -1.550809 | 5.295667 | 1169.4386 | 1185.2176 | 1229.9302 |
| | H | -0.956608 | -1.657890 | 5.309472 | 1243.3536 | 1292.5982 | 1321.1335 |
| | H | 0.372183 | -0.710307 | 5.955624 | 1326.7313 | 1330.0786 | 1387.9157 |
| | C | 0.791145 | -2.824884 | 5.819066 | 1395.0703 | 1404.3215 | 1417.1464 |
| | H | 0.545825 | -3.681717 | 5.185270 | 1483.379 | 1487.5844 | 1497.4328 |
| | H | 1.879224 | -2.723367 | 5.839446 | 1506.9947 | 1511.8281 | 1524.2785 |
| | H | 0.462424 | -3.055185 | 6.832789 | 1647.2366 | 1659.298 | 1674.2911 |
| | H | 0.208610 | 0.795618 | 3.887084 | 1848.5714 | 3035.9956 | 3050.7925 |
| | H | -1.012945 | -0.082747 | 3.282211 | 3058.437 | 3068.8062 | 3094.1628 |
| | H | 3.594355 | 0.000740 | 1.401928 | 3125.0003 | 3149.1638 | 3209.3171 |
| | C | -0.047070 | -2.546507 | 0.223916 | 3218.635 | 3228.7222 | 3235.1754 |
| | O | 0.480889 | -3.527374 | -0.230244 | 3515.465 | 3592.9361 | 3829.6038 |
| | O | -1.271923 | -2.563192 | 0.765188 | | | |
| | H | -1.600008 | -3.471767 | 0.718796 | | | |
| TS (-0.006) | C | 0.000000 | 0.000000 | 0.000000 | -335.3152 | 39.4367 | 52.3929 |
| | N | 0.000000 | 0.000000 | 1.874757 | 66.9057 | 83.6002 | 112.5679 |
| | C | 2.454196 | 0.000000 | -1.474928 | 147.648 | 163.3857 | 191.2558 |
| | C | 1.803508 | -1.177594 | -1.179605 | 221.6567 | 234.5257 | 255.8763 |
| | C | 1.845852 | 1.202477 | -1.068129 | 298.2715 | 319.8396 | 356.5791 |
| | H | 2.212341 | -2.134879 | -1.483825 | 408.0587 | 442.9641 | 448.9751 |
| | H | 2.311150 | 2.152827 | -1.309286 | 517.4533 | 542.7061 | 590.6543 |
| | C | 0.594177 | -1.215023 | -0.468974 | 630.5972 | 646.9236 | 683.7095 |
| | C | 0.654124 | 1.217348 | -0.390602 | 729.3775 | 740.8255 | 755.7905 |
| | H | 0.175692 | 2.153975 | -0.129562 | 785.7496 | 817.6948 | 844.2299 |
| | Cl | -1.832210 | 0.134113 | -0.116706 | 886.8904 | 913.9078 | 978.3159 |
| | C | 1.348190 | -0.241924 | 2.405026 | 988.4325 | 1000.262 | 1048.7647 |
| | H | 1.642137 | -1.242233 | 2.076295 | 1053.5996 | 1057.4083 | 1091.1431 |
| | H | 2.016831 | 0.474829 | 1.917615 | 1096.7657 | 1110.743 | 1132.2447 |
| | C | 1.433016 | -0.125714 | 3.923516 | 1171.6712 | 1181.5911 | 1211.6356 |
| | H | 0.733931 | -0.832383 | 4.380961 | 1236.2843 | 1275.3068 | 1326.9525 |
| | H | 1.116334 | 0.876479 | 4.229548 | 1330.1043 | 1340.7366 | 1384.5119 |
| | C | 2.849738 | -0.397833 | 4.423090 | 1391.089 | 1410.0645 | 1423.0903 |
| | H | 3.172700 | -1.406176 | 4.154272 | 1450.3615 | 1492.8792 | 1498.461 |
| | H | 3.560071 | 0.312414 | 3.993314 | 1501.2097 | 1507.595 | 1515.6656 |
| | H | 2.902940 | -0.308959 | 5.507974 | 1582.1777 | 1627.3881 | 1664.1881 |
| | H | -0.369086 | 0.905826 | 2.161827 | 1819.2578 | 3056.9698 | 3066.1086 |
| | H | -0.657660 | -0.725715 | 2.159732 | 3071.7181 | 3093.6695 | 3123.7661 |
| | H | 3.397891 | 0.002341 | -2.002951 | 3137.1071 | 3157.3037 | 3189.5808 |
| | C | 0.044727 | -2.542821 | -0.176681 | 3209.2152 | 3212.2023 | 3237.1379 |
| | O | 0.312021 | -3.563624 | -0.764044 | 3481.4224 | 3573.3678 | 3837.9299 |
| | O | -0.787208 | -2.553481 | 0.898218 | | | |
| | H | -1.088651 | -3.463938 | 1.017854 | | | |
| PC (-0.006) | C | 0.0000 | 0.0000 | 0.0000 | 16.9244 | 38.3192 | 44.4642 |
| | N | 0.0000 | 0.0000 | 1.376293 | 59.7121 | 86.7737 | 96.2194 |
| | C | 0.2096 | 0.0000 | -2.828553 | 104.7915 | 145.4574 | 178.0109 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|-------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | C | -0.543848 | 0.955961 | -2.17603 | 231.7833 | 240.5609 | 261.8479 |
| | C | 0.85782 | -0.969747 | -2.063178 | 298.8873 | 314.7873 | 400.044 |
| | H | -1.066475 | 1.727906 | -2.727333 | 430.2487 | 443.38 | 512.2654 |
| | H | 1.457308 | -1.734692 | -2.544272 | 533.6316 | 570.9454 | 577.5703 |
| | C | -0.666205 | 0.980689 | -0.782638 | 591.8825 | 630.9126 | 647.6735 |
| | C | 0.755187 | -0.974897 | -0.685995 | 652.9459 | 722.486 | 764.7833 |
| | H | 1.275579 | -1.733738 | -0.119135 | 773.2263 | 775.8589 | 812.6323 |
| | Cl | 2.766442 | 1.626269 | 1.267413 | 868.1883 | 873.65 | 919.2574 |
| | C | 0.507176 | -1.119237 | 2.169527 | 932.8623 | 989.6314 | 1000.0363 |
| | H | 0.013134 | -2.055048 | 1.877428 | 1065.8482 | 1077.9662 | 1099.4759 |
| | H | 1.58039 | -1.233779 | 1.98004 | 1117.8419 | 1145.0559 | 1169.4066 |
| | C | 0.288998 | -0.845043 | 3.651678 | 1179.1447 | 1191.3047 | 1220.0894 |
| | H | -0.781327 | -0.709327 | 3.83939 | 1280.2618 | 1288.0783 | 1310.4698 |
| | H | 0.784374 | 0.094722 | 3.915032 | 1326.5512 | 1336.3571 | 1358.3083 |
| | C | 0.82776 | -1.979203 | 4.51815 | 1390.858 | 1416.3956 | 1423.8229 |
| | H | 0.334937 | -2.924986 | 4.280868 | 1487.247 | 1496.7866 | 1507.9639 |
| | H | 1.902412 | -2.107776 | 4.370802 | 1509.299 | 1513.5162 | 1531.9226 |
| | H | 0.660896 | -1.773681 | 5.575217 | 1563.072 | 1644.9301 | 1683.0195 |
| | H | 1.569754 | 1.151656 | 1.480987 | 1833.5487 | 2610.706 | 3025.0632 |
| | H | -0.720851 | 0.551787 | 1.820591 | 3054.9593 | 3067.3558 | 3070.5106 |
| | H | 0.293958 | 0.005222 | -3.907977 | 3099.6969 | 3136.8043 | 3157.9911 |
| | C | -1.509257 | 2.086867 | -0.259333 | 3198.0752 | 3215.175 | 3228.8886 |
| | O | -2.051892 | 2.913231 | -0.947486 | 3248.6339 | 3626.6205 | 3825.9507 |
| | O | -1.636787 | 2.103333 | 1.08375 | | | |
| | H | -2.186437 | 2.862892 | 1.322927 | | | |
| 2-chlorobenzoic acid (-0.010) | C | 0.000000 | 0.000000 | 0.000000 | 4.9417 | 114.762 | 214.1966 |
| | Cl | 0.000000 | 0.000000 | 1.722390 | 219.3299 | 304.1634 | 351.4861 |
| | C | 0.266731 | 0.000000 | -2.787781 | 430.9278 | 472.6278 | 507.6889 |
| | C | -0.984344 | -0.005551 | -2.198747 | 533.5342 | 611.9364 | 641.7245 |
| | C | 1.399759 | 0.005922 | -1.976398 | 703.9793 | 715.607 | 758.4278 |
| | H | -1.887125 | -0.009972 | -2.796589 | 806.9661 | 818.6788 | 892.8019 |
| | H | 2.393308 | 0.010453 | -2.409972 | 986.9363 | 999.8944 | 1075.5407 |
| | C | -1.147936 | -0.005785 | -0.807609 | 1082.3245 | 1154.1533 | 1168.8804 |
| | C | 1.264536 | 0.005936 | -0.599957 | 1180.31 | 1215.9622 | 1284.1762 |
| | H | 2.135057 | 0.010369 | 0.043502 | 1321.9765 | 1415.0041 | 1479.8997 |
| | H | 0.361025 | -0.000158 | -3.867783 | 1516.4943 | 1633.1554 | 1670.6019 |
| | C | -2.580160 | -0.012474 | -0.349885 | 1821.6366 | 3191.0907 | 3209.6014 |
| | O | -3.502080 | -0.014193 | -1.130411 | 3228.4514 | 3231.4271 | 3815.9394 |
| | O | -2.734406 | -0.016603 | 0.963385 | | | |
| | H | -3.679199 | -0.020741 | 1.175633 | | | |
| Propylamine (-0.010) | N | 0.000000 | 0.000000 | 0.000000 | 128.9411 | 230.0102 | 272.3814 |
| | C | 0.000000 | 0.000000 | 2.535457 | 292.7058 | 452.3395 | 747.7151 |
| | C | 0.803310 | 0.000000 | 1.236339 | 865.9037 | 877.6833 | 963.4987 |
| | H | 1.458156 | -0.876264 | 1.21004 | 1038.0699 | 1050.9308 | 1098.0137 |
| | H | 1.458025 | 0.876358 | 1.209932 | 1151.1402 | 1241.139 | 1325.0019 |
| | H | -0.655062 | -0.878592 | 2.550421 | 1325.8333 | 1389.4022 | 1399.811 |
| | H | -0.654112 | 0.879293 | 2.550914 | 1423.1198 | 1487.777 | 1499.5493 |
| | C | 0.898030 | -0.000794 | 3.770363 | 1505.9102 | 1512.8186 | 1661.9705 |
| | H | 1.540352 | -0.884420 | 3.788371 | 3039.7158 | 3059.7942 | 3067.0919 |
| | H | 1.541167 | 0.882232 | 3.788865 | 3071.8998 | 3104.5427 | 3134.274 |
| | H | 0.312161 | -0.000767 | 4.689283 | 3157.4987 | 3504.9035 | 3578.8836 |
| | H | -0.618471 | 0.806673 | 0.025978 | | | |
| | H | -0.618429 | -0.806706 | 0.025891 | | | |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|-------------|---------------------------|-----------|-----------|------------------------------|-----------|-----------|-----------|
| RC (-0.010) | C | 0.000000 | 0.000000 | 0.000000 | 12.7399 | 28.1896 | 30.0177 |
| | N | 0.000000 | 0.000000 | 3.378961 | 39.2105 | 54.656 | 56.7682 |
| | C | 2.519220 | 0.000000 | 1.149505 | 108.2121 | 128.0091 | 135.7037 |
| | C | 1.890795 | -1.201635 | 0.855515 | 161.162 | 197.286 | 232.3564 |
| | C | 1.882334 | 1.201013 | 0.860793 | 282.9453 | 290.2026 | 293.0281 |
| | H | 2.363931 | -2.146296 | 1.097288 | 349.7304 | 389.7884 | 450.8281 |
| | H | 2.354058 | 2.141668 | 1.118334 | 455.6339 | 464.8155 | 570.8095 |
| | C | 0.615432 | -1.211165 | 0.294870 | 592.8873 | 639.5181 | 699.1285 |
| | C | 0.626380 | 1.206559 | 0.267276 | 736.3644 | 745.0099 | 771.141 |
| | H | 0.114342 | 2.134977 | 0.049762 | 797.4505 | 810.2046 | 865.4662 |
| | Cl | -1.577156 | 0.027132 | -0.763093 | 879.5932 | 889.7686 | 964.864 |
| | C | 0.722632 | -1.110879 | 4.014347 | 979.6507 | 1019.6352 | 1038.6098 |
| | H | 0.556334 | -2.007580 | 3.403652 | 1053.2784 | 1058.0717 | 1071.2931 |
| | H | 1.794885 | -0.891027 | 3.952970 | 1106.1199 | 1151.4686 | 1157.8136 |
| | C | 0.348143 | -1.406422 | 5.464640 | 1170.9507 | 1185.7886 | 1230.1165 |
| | H | -0.724204 | -1.623236 | 5.519593 | 1241.1566 | 1291.5914 | 1319.2232 |
| | H | 0.514289 | -0.507536 | 6.067037 | 1323.8961 | 1327.6597 | 1387.2165 |
| | C | 1.147179 | -2.570938 | 6.043014 | 1397.363 | 1398.0386 | 1418.3383 |
| | H | 0.975924 | -3.488080 | 5.471978 | 1482.716 | 1485.723 | 1495.4921 |
| | H | 2.218971 | -2.357390 | 6.027909 | 1507.4408 | 1510.4362 | 1524.7089 |
| | H | 0.867591 | -2.767248 | 7.077985 | 1647.5554 | 1662.5177 | 1675.4646 |
| | H | 0.143307 | 0.840292 | 3.933539 | 1844.4469 | 3028.2734 | 3052.2306 |
| | H | -0.997860 | -0.187278 | 3.435779 | 3058.1221 | 3065.0145 | 3095.2501 |
| | H | 3.488117 | 0.000005 | 1.633189 | 3124.9141 | 3154.9785 | 3209.7837 |
| | C | -0.045895 | -2.533347 | 0.075129 | 3216.8519 | 3229.0679 | 3235.395 |
| | O | 0.389666 | -3.405010 | -0.633140 | 3510.5726 | 3583.2624 | 3828.3336 |
| | O | -1.162600 | -2.659952 | 0.795006 | | | |
| | H | -1.508606 | -3.554262 | 0.668526 | | | |
| TS (-0.010) | C | 0.000000 | 0.000000 | 0.000000 | -309.5276 | 35.0721 | 50.6242 |
| | N | 0.000000 | 0.000000 | 1.932444 | 65.1728 | 83.7615 | 109.5994 |
| | C | 2.499974 | 0.000000 | -1.386647 | 143.4761 | 163.2368 | 185.5773 |
| | C | 1.830979 | -1.177540 | -1.127803 | 216.7118 | 230.4216 | 249.3214 |
| | C | 1.884152 | 1.202628 | -0.992555 | 295.8392 | 322.6757 | 351.3255 |
| | H | 2.249199 | -2.134862 | -1.419154 | 411.3036 | 436.9473 | 445.5818 |
| | H | 2.368965 | 2.152217 | -1.195753 | 512.0394 | 545.322 | 598.316 |
| | C | 0.595228 | -1.211671 | -0.466750 | 628.476 | 650.943 | 655.9734 |
| | C | 0.664788 | 1.216616 | -0.364796 | 729.2999 | 739.2654 | 753.0945 |
| | H | 0.186874 | 2.152461 | -0.100562 | 788.7549 | 818.151 | 846.3715 |
| | Cl | -1.816514 | 0.132520 | -0.110333 | 881.757 | 911.5107 | 980.222 |
| | C | 1.341408 | -0.267376 | 2.469695 | 993.1379 | 998.1661 | 1043.3803 |
| | H | 1.626236 | -1.266979 | 2.128961 | 1052.5026 | 1055.7984 | 1079.0029 |
| | H | 2.024441 | 0.449137 | 2.001520 | 1091.2617 | 1110.1826 | 1141.326 |
| | C | 1.416703 | -0.176989 | 3.991837 | 1164.7426 | 1180.9268 | 1211.7791 |
| | H | 0.705319 | -0.882211 | 4.431996 | 1234.7435 | 1274.4638 | 1328.3972 |
| | H | 1.108520 | 0.823443 | 4.311477 | 1330.185 | 1337.8573 | 1382.3104 |
| | C | 2.824876 | -0.473787 | 4.500991 | 1393.2276 | 1402.6419 | 1423.6251 |
| | H | 3.139249 | -1.482204 | 4.221958 | 1452.6971 | 1491.1553 | 1498.6336 |
| | H | 3.548441 | 0.236379 | 4.093339 | 1499.9722 | 1507.0776 | 1514.2805 |
| | H | 2.865373 | -0.403077 | 5.587579 | 1584.9434 | 1630.1729 | 1662.4975 |
| | H | -0.350423 | 0.910882 | 2.227713 | 1812.3273 | 3057.506 | 3063.9358 |
| | H | -0.669792 | -0.709456 | 2.229150 | 3069.0738 | 3094.5399 | 3118.3304 |
| | H | 3.472566 | -0.000385 | -1.860327 | 3136.1142 | 3160.1559 | 3187.9568 |
| | C | 0.019865 | -2.540593 | -0.213496 | 3206.5694 | 3213.6741 | 3230.3498 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|--------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | O | 0.256379 | -3.538880 | -0.854145 | 3482.058 | 3571.8629 | 3833.8941 |
| | O | -0.786618 | -2.569873 | 0.870026 | | | |
| | H | -1.091881 | -3.479229 | 0.991485 | | | |
| PC (-0.010) | C | 0.000000 | 0.000000 | 0.000000 | 24.39 | 34.112 | 46.0073 |
| | N | 0.000000 | 0.000000 | 1.360377 | 61.792 | 79.9474 | 94.5304 |
| | C | 0.216550 | 0.000000 | -2.837216 | 102.6095 | 140.6577 | 174.324 |
| | C | -0.687716 | 0.822097 | -2.194529 | 230.6147 | 237.6843 | 255.8221 |
| | C | 1.011254 | -0.844830 | -2.055990 | 296.3443 | 315.1607 | 392.7059 |
| | H | -1.329260 | 1.493161 | -2.752970 | 401.9861 | 429.279 | 450.9661 |
| | H | 1.730629 | -1.508078 | -2.524932 | 458.2678 | 545.837 | 565.0174 |
| | C | -0.820383 | 0.844638 | -0.802032 | 590.2354 | 601.132 | 627.3322 |
| | C | 0.905123 | -0.852630 | -0.682603 | 647.018 | 715.9833 | 749.3485 |
| | H | 1.537945 | -1.510917 | -0.104354 | 769.5419 | 774.912 | 808.7947 |
| | Cl | 2.304486 | 2.346375 | 0.595721 | 856.4862 | 869.4562 | 916.6392 |
| | C | 0.767921 | -0.929234 | 2.189654 | 929.8324 | 978.7868 | 986.6515 |
| | H | 0.497776 | -1.965341 | 1.949604 | 1063.9687 | 1072.7223 | 1095.2381 |
| | H | 1.836421 | -0.804740 | 1.977465 | 1113.4965 | 1146.2095 | 1166.116 |
| | C | 0.508171 | -0.649125 | 3.664900 | 1175.9189 | 1191.1218 | 1216.2199 |
| | H | -0.562053 | -0.758455 | 3.867968 | 1277.1559 | 1285.8201 | 1313.7904 |
| | H | 0.772955 | 0.390444 | 3.883124 | 1322.0167 | 1332.422 | 1365.6648 |
| | C | 1.304316 | -1.588159 | 4.566178 | 1397.5479 | 1413.6691 | 1426.1289 |
| | H | 1.036757 | -2.631487 | 4.384070 | 1486.4867 | 1495.7813 | 1507.5088 |
| | H | 2.378376 | -1.474934 | 4.402771 | 1507.8809 | 1515.9963 | 1530.5616 |
| | H | 1.106896 | -1.375511 | 5.616298 | 1565.7461 | 1638.806 | 1682.293 |
| | H | 1.418691 | 1.678211 | 1.260835 | 1820.4162 | 2824.04 | 3025.6506 |
| | H | -0.749379 | 0.492823 | 1.825265 | 3056.8548 | 3064.1341 | 3069.7565 |
| | H | 0.304002 | 0.010244 | -3.917213 | 3100.2494 | 3138.99 | 3162.5691 |
| | C | -1.827687 | 1.809640 | -0.295174 | 3185.36 | 3204.4298 | 3223.3388 |
| | O | -2.527999 | 2.495561 | -0.999735 | 3249.0998 | 3632.5172 | 3817.6824 |
| | O | -1.905195 | 1.868823 | 1.046140 | | | |
| | H | -2.572727 | 2.525312 | 1.292246 | | | |
| 2-chlorobenzoic acid (-0.0175) | C | 0.000000 | 0.000000 | 0.000000 | 28.5186 | 111.4215 | 210.7742 |
| | Cl | 0.000000 | 0.000000 | 1.711063 | 220.8885 | 308.8017 | 352.3595 |
| | C | 0.288881 | 0.000000 | -2.796170 | 423.02 | 474.1604 | 503.6486 |
| | C | -0.965524 | 0.001794 | -2.213519 | 535.3387 | 625.1173 | 639.7071 |
| | C | 1.416964 | -0.001889 | -1.973597 | 691.7148 | 716.6184 | 733.8833 |
| | H | -1.867825 | 0.003211 | -2.813208 | 807.562 | 807.5974 | 868.9894 |
| | H | 2.416288 | -0.003303 | -2.395713 | 947.5497 | 979.0503 | 1070.4941 |
| | C | -1.140019 | 0.001838 | -0.823343 | 1084.9728 | 1149.7996 | 1166.2474 |
| | C | 1.270575 | -0.001956 | -0.600037 | 1179.0735 | 1200.7913 | 1278.9739 |
| | H | 2.135802 | -0.003341 | 0.051447 | 1325.4373 | 1421.9849 | 1478.7308 |
| | H | 0.391310 | 0.000402 | -3.877864 | 1511.5104 | 1623.5566 | 1666.578 |
| | C | -2.579344 | 0.00338 | -0.375306 | 1806.2805 | 3158.184 | 3195.5597 |
| | O | -3.490941 | 0.003482 | -1.174016 | 3217.6771 | 3225.6207 | 3801.0508 |
| | O | -2.72839 | 0.00475 | 0.92848 | | | |
| | H | -3.665101 | 0.005845 | 1.17947 | | | |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|-----------------------|---------------------------|-----------|-----------|------------------------------|-------------|-------------|-----------|
| Propylamine (-0.0175) | N | 0.000000 | 0.000000 | 0.000000 | 128.354000 | 231.327100 | 273.3056 |
| | C | 0.000000 | 0.000000 | 2.536014 | 308.389400 | 451.705500 | 748.4757 |
| | C | 0.812691 | 0.000000 | 1.243367 | 867.646200 | 884.147100 | 989.0092 |
| | H | 1.465402 | -0.877543 | 1.216313 | 1037.820400 | 1047.807400 | 1082.8225 |
| | H | 1.465045 | 0.877804 | 1.216045 | 1158.227400 | 1239.267500 | 1321.1989 |
| | H | -0.655402 | -0.878979 | 2.545469 | 1322.760000 | 1387.320800 | 1390.2928 |
| | H | -0.653090 | 0.880683 | 2.546777 | 1426.955900 | 1485.598800 | 1498.0445 |
| | C | 0.885470 | -0.001968 | 3.781175 | 1504.479200 | 1511.775700 | 1659.9555 |
| | H | 1.524995 | -0.886982 | 3.810223 | 3035.437000 | 3061.543200 | 3068.9494 |
| | H | 1.526692 | 0.881776 | 3.811629 | 3070.637900 | 3106.994800 | 3139.4513 |
| | H | 0.288253 | -0.002065 | 4.692524 | 3163.008900 | 3490.262200 | 3557.9505 |
| | H | -0.624853 | 0.801444 | 0.064336 | | | |
| | H | -0.625040 | -0.801298 | 0.064341 | | | |
| RC (-0.0175) | C | 0.000000 | 0.000000 | 0.000000 | -9.0864 | 36.1378 | 44.4869 |
| | N | 0.000000 | 0.000000 | 3.297188 | 58.6486 | 64.1296 | 72.2601 |
| | C | 2.411927 | 0.000000 | 1.372973 | 125.8064 | 142.6562 | 154.9745 |
| | C | 1.799401 | -1.197215 | 1.036498 | 178.1447 | 215.5727 | 231.2276 |
| | C | 1.792031 | 1.200117 | 1.049756 | 295.246 | 296.4064 | 311.9752 |
| | H | 2.229527 | -2.138485 | 1.357375 | 355.5399 | 391.6811 | 449.4471 |
| | H | 2.221184 | 2.138323 | 1.381573 | 456.0533 | 459.7636 | 557.5061 |
| | C | 0.602313 | -1.215259 | 0.314524 | 593.6757 | 636.7261 | 694.4394 |
| | C | 0.577981 | 1.203120 | 0.373271 | 705.2342 | 748.8071 | 762.6715 |
| | H | 0.051082 | 2.129448 | 0.182664 | 799.4391 | 814.1477 | 868.5027 |
| | Cl | -1.532459 | 0.066692 | -0.859741 | 885.5419 | 888.3878 | 980.5617 |
| | C | 1.107873 | 0.102853 | 4.276792 | 996.4659 | 1016.3111 | 1035.9912 |
| | H | 1.788446 | -0.739557 | 4.099909 | 1052.3269 | 1053.7798 | 1076.1597 |
| | H | 1.674476 | 1.014776 | 4.047005 | 1089.8705 | 1157.9658 | 1162.5957 |
| | C | 0.691729 | 0.118661 | 5.744891 | 1175.4706 | 1189.68 | 1204.5457 |
| | H | 0.121269 | -0.790526 | 5.963443 | 1240.4381 | 1293.5163 | 1321.7565 |
| | H | 0.012748 | 0.961408 | 5.915011 | 1322.6296 | 1326.3754 | 1383.5958 |
| | C | 1.887481 | 0.218498 | 6.688996 | 1389.4403 | 1397.7105 | 1424.0377 |
| | H | 2.561940 | -0.632597 | 6.565624 | 1475.9203 | 1484.4981 | 1494.143 |
| | H | 2.454829 | 1.136588 | 6.515703 | 1504.7716 | 1508.9833 | 1525.2215 |
| | H | 1.565107 | 0.227918 | 7.729992 | 1641.577 | 1661.3549 | 1671.2969 |
| | H | -0.658308 | 0.744923 | 3.521113 | 1806.056 | 3020.1491 | 3049.9088 |
| | H | -0.517777 | -0.846100 | 3.530757 | 3055.166 | 3063.5626 | 3092.2815 |
| | H | 3.322872 | -0.005547 | 1.958584 | 3131.1973 | 3160.5044 | 3211.2572 |
| | C | 0.017972 | -2.533799 | -0.06016 | 3220.8946 | 3229.0879 | 3235.3962 |
| O | -0.455703 | -2.822457 | -1.138343 | 3486.8001 | 3548.8287 | 3847.3625 | |
| O | 0.123216 | -3.402097 | 0.942585 | | | | |
| H | -0.282061 | -4.242803 | 0.693419 | | | | |
| TS (-0.0175) | C | 0.000000 | 0.000000 | 0.000000 | -233.468 | 22.6941 | 48.0146 |
| | N | 0.000000 | 0.000000 | 2.087835 | 58.5236 | 81.7911 | 106.5849 |
| | C | 2.575054 | 0.000000 | -1.207323 | 132.8937 | 160.6251 | 171.4699 |
| | C | 1.875878 | -1.177539 | -1.026480 | 200.1807 | 216.2418 | 241.74 |
| | C | 1.951754 | 1.202435 | -0.826230 | 291.1478 | 312.5304 | 349.3123 |
| | H | 2.311517 | -2.133505 | -1.296592 | 418.1114 | 426.5145 | 437.0462 |
| | H | 2.474232 | 2.146735 | -0.941968 | 496.4155 | 539.9741 | 573.8967 |
| | C | 0.596216 | -1.204461 | -0.458221 | 606.0616 | 637.1442 | 661.7208 |
| | C | 0.68611 | 1.215042 | -0.293022 | 724.9077 | 740.3549 | 748.3486 |
| | H | 0.210903 | 2.146572 | -0.010153 | 794.5668 | 818.2551 | 852.7311 |
| | Cl | -1.789786 | 0.127172 | -0.074204 | 874.5346 | 903.9657 | 969.0852 |
| | C | 1.326671 | -0.303221 | 2.649492 | 995.584 | 1019.5901 | 1031.4666 |

| | Solvent (Toluene) | | | | | | |
|----------------------|---------------------------|-----------|-----------|-------------------------------|-------------|-------------|-------------|
| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
| | H | 1.612581 | -1.294898 | 2.282223 | 1048.4379 | 1053.4201 | 1059.4764 |
| | H | 2.032869 | 0.423298 | 2.231761 | 1078.1011 | 1116.5628 | 1153.0786 |
| | C | 1.366233 | -0.271386 | 4.178875 | 1155.1213 | 1180.6287 | 1207.6407 |
| | H | 0.63625 | -0.985111 | 4.572718 | 1232.5555 | 1273.394 | 1325.8811 |
| | H | 1.05646 | 0.718828 | 4.527209 | 1328.6962 | 1331.3974 | 1376.3231 |
| | C | 2.755339 | -0.599725 | 4.719801 | 1385.7457 | 1400.978200 | 1424.659200 |
| | H | 3.071442 | -1.601399 | 4.417962 | 1458.3696 | 1486.226600 | 1494.610000 |
| | H | 3.497893 | 0.121768 | 4.369466 | 1499.3934 | 1505.859900 | 1510.581600 |
| | H | 2.75739 | -0.570203 | 5.809399 | 1590.973500 | 1635.854700 | 1657.162200 |
| | H | -0.324814 | 0.913238 | 2.406481 | 1793.060600 | 3045.814900 | 3059.256100 |
| | H | -0.684932 | -0.68457 | 2.407745 | 3066.821800 | 3086.509800 | 3108.715200 |
| | H | 3.593297 | -0.006841 | -1.575336 | 3133.288700 | 3158.950000 | 3184.914000 |
| | C | -0.026693 | -2.533064 | -0.285123 | 3201.132300 | 3216.149400 | 3222.276600 |
| | O | 0.14445 | -3.47258 | -1.034666 | 3478.132900 | 3562.530400 | 3825.692600 |
| | O | -0.774761 | -2.612280 | 0.818123 | | | |
| | H | -1.092851 | -3.518876 | 0.933292 | | | |
| Propylamine | C | -0.588819 | -0.509894 | -0.000083 | 126.300900 | 226.5013 | 267.012 |
| | H | -0.481686 | -1.157382 | 0.875936 | 269.227100 | 450.0175 | 743.0976 |
| | H | -0.481618 | -1.157215 | -0.876216 | 851.860100 | 860.0187 | 921.5206 |
| | C | 0.532356 | 0.529891 | 0.000041 | 1033.709400 | 1051.23 | 1110.8352 |
| | H | 0.419537 | 1.174176 | 0.878903 | 1146.113500 | 1239.4742 | 1324.8581 |
| | H | 0.419595 | 1.174316 | -0.878730 | 1326.134900 | 1387.1873 | 1403.7155 |
| | C | 1.915877 | -0.116150 | 0.000020 | 1409.501800 | 1482.7964 | 1495.8914 |
| | H | 2.050718 | -0.746753 | 0.882703 | 1500.95 | 1509.1137 | 1657.519 |
| | H | 2.050654 | -0.746824 | -0.882625 | 3043.1373 | 3055.087 | 3058.2209 |
| | H | 2.708786 | 0.633688 | -0.000041 | 3074.047 | 3100.4617 | 3125.5313 |
| | N | -1.950724 | 0.024623 | -0.000069 | 3136.6759 | 3526.7045 | 3606.5624 |
| | H | -2.093480 | 0.615897 | -0.812867 | | | |
| | H | -2.093927 | 0.614654 | 0.813550 | | | |
| 2-chlorobenzoic acid | C | 2.156746 | -1.457885 | 0.082909 | 36.3246 | 115.085100 | 201.664400 |
| | C | 0.783908 | -1.638157 | 0.03633 | 208.239 | 298.681600 | 345.616000 |
| | C | 2.677509 | -0.167844 | 0.077668 | 420.1718 | 461.293200 | 489.671 |
| | H | 0.354408 | -2.632232 | 0.030483 | 548.084600 | 583.876900 | 640.2635 |
| | H | 3.748495 | -0.008696 | 0.110557 | 701.747900 | 718.771300 | 772.9913 |
| | C | -0.091794 | -0.548316 | 0.002671 | 802.071300 | 821.520300 | 905.4273 |
| | C | 1.827676 | 0.928086 | 0.017421 | 999.202400 | 1027.686200 | 1066.132 |
| | H | 2.222871 | 1.935238 | -0.009908 | 1074.825700 | 1153.955500 | 1165.774 |
| | C | 0.449473 | 0.741376 | -0.017015 | 1184.939100 | 1228.135200 | 1291.2798 |
| | Cl | -0.530944 | 2.173787 | -0.156783 | 1316.4602 | 1399.1009 | 1480.8527 |
| | H | 2.815338 | -2.316149 | 0.120197 | 1520.4381 | 1640.2763 | 1668.1662 |
| | C | -1.546239 | -0.896883 | -0.015611 | 1829.8532 | 3213.9816 | 3223.7707 |
| | O | -1.967028 | -1.9248 | -0.479848 | 3232.7547 | 3237.9977 | 3817.4647 |
| | O | -2.334671 | 0.002983 | 0.578475 | | | |
| | H | -3.24514 | -0.320276 | 0.51873 | | | |
| TS | C | -1.148915 | 2.325252 | -1.360618 | -366.8663 | 39.5416 | 57.1759 |
| | C | -1.282654 | 0.983358 | -1.630715 | 68.7327 | 82.2536 | 113.2061 |
| | C | -0.826698 | 2.699541 | -0.041435 | 149.8194 | 166.4749 | 194.5887 |
| | H | -1.551817 | 0.638968 | -2.622974 | 224.6952 | 234.8909 | 262.1866 |
| | H | -0.753388 | 3.750441 | 0.218294 | 301.4249 | 310.8842 | 358.7725 |
| | C | -1.082325 | -0.009569 | -0.654868 | 405.9071 | 445.3056 | 451.7191 |
| | C | -0.636810 | 1.771146 | 0.949292 | 519.0007 | 535.3121 | 570.6779 |
| | H | -0.447836 | 2.080945 | 1.970324 | 627.8641 | 641.2207 | 700.4649 |
| | C | -0.713713 | 0.363641 | 0.678102 | 726.5737 | 746.0109 | 755.5881 |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|----------------------------------|---------------------------|-----------|-----------|------------------------------|------------|-----------|-----------|
| | Cl | -1.534831 | -0.552572 | 2.069773 | 783.4349 | 817.0824 | 844.9312 |
| | C | 1.929906 | 0.075911 | 0.039487 | 888.2303 | 912.3384 | 962.9646 |
| | H | 1.597298 | -0.346831 | -0.911857 | 993.8052 | 1006.5459 | 1048.11 |
| | H | 1.859288 | 1.164891 | -0.042739 | 1053.907 | 1058.759 | 1090.8108 |
| | C | 3.357639 | -0.358268 | 0.350671 | 1100.9622 | 1111.7062 | 1124.0984 |
| | H | 3.389513 | -1.447144 | 0.455216 | 1172.8248 | 1182.5773 | 1207.4705 |
| | H | 3.664784 | 0.064432 | 1.312468 | 1235.2955 | 1273.8002 | 1323.3601 |
| | C | 4.320263 | 0.090416 | -0.746426 | 1329.0963 | 1340.4829 | 1384.1142 |
| | H | 4.041045 | -0.341430 | -1.710211 | 1390.4677 | 1413.2977 | 1415.7102 |
| | H | 4.312589 | 1.177866 | -0.850854 | 1448.6284 | 1488.2877 | 1494.5068 |
| | H | 5.341521 | -0.219352 | -0.521546 | 1498.8917 | 1500.6321 | 1513.3355 |
| | N | 0.955858 | -0.340408 | 1.053952 | 1580.6261 | 1625.9656 | 1662.6287 |
| | H | 1.198000 | -0.008412 | 1.986631 | 1797.7236 | 3055.8932 | 3064.2845 |
| | H | 0.832570 | -1.352222 | 1.081715 | 3074.1789 | 3092.2678 | 3126.1249 |
| | H | -1.309314 | 3.070145 | -2.127554 | 3136.6064 | 3146.552 | 3194.3935 |
| | C | -1.191574 | -1.398264 | -1.099479 | 3212.802 | 3214.9713 | 3241.3858 |
| | O | -1.688418 | -1.777547 | -2.134568 | 3484.1369 | 3577.5435 | 3831.0677 |
| | O | -0.607372 | -2.290454 | -0.250869 | | | |
| | H | -0.757513 | -3.170702 | -0.62129 | | | |
| Propylamine (-0.006) | N | -0.002348 | -0.000090 | -0.008007 | 128.722100 | 226.9672 | 270.9938 |
| | C | 0.008371 | -0.000033 | 2.523208 | 283.579000 | 451.5381 | 746.6011 |
| | C | 0.807446 | -0.000025 | 1.221284 | 865.839 | 875.2831 | 956.5249 |
| | H | 1.462259 | -0.876492 | 1.194499 | 1038.1772 | 1052.9616 | 1100.2992 |
| | H | 1.462184 | 0.876495 | 1.194463 | 1150.5956 | 1240.5316 | 1326.7108 |
| | H | -0.646180 | -0.878847 | 2.537399 | 1326.9006 | 1387.9733 | 1401.8496 |
| | H | -0.646227 | 0.878747 | 2.537385 | 1416.2749 | 1482.6376 | 1496.4703 |
| | C | 0.904999 | 0.000004 | 3.758330 | 1499.9762 | 1509.7624 | 1655.1914 |
| | H | 1.547711 | -0.883475 | 3.776436 | 3040.4451 | 3058.0893 | 3064.0013 |
| | H | 1.547699 | 0.883493 | 3.776396 | 3072.456 | 3102.785 | 3131.2799 |
| | H | 0.316253 | 0.000021 | 4.675902 | 3151.0765 | 3510.0713 | 3584.2097 |
| | H | -0.619313 | 0.807531 | 0.012271 | | | |
| | H | -0.618898 | -0.808031 | 0.012099 | | | |
| 2-chlorobenzoic acid (-0.006) | C | -0.025296 | -0.028712 | 0.003539 | 30.858 | 115.4573 | 208.9585 |
| | Cl | -0.043707 | -0.088932 | 1.731377 | 216.1625 | 302.9929 | 348.4407 |
| | C | 0.227311 | 0.022395 | -2.778896 | 426.6751 | 468.1215 | 498.3796 |
| | C | -0.783824 | 0.729166 | -2.15148 | 542.6156 | 598.076 | 640.3713 |
| | C | 1.119891 | -0.718784 | -2.008491 | 705.3842 | 715.2288 | 762.3718 |
| | H | -1.488084 | 1.321592 | -2.721889 | 804.6401 | 820.9537 | 896.7173 |
| | H | 1.921156 | -1.278158 | -2.476863 | 991.1304 | 1010.5865 | 1074.4663 |
| | C | -0.938554 | 0.711183 | -0.760734 | 1076.89 | 1153.5077 | 1167.7928 |
| | C | 0.997167 | -0.738476 | -0.628483 | 1177.9946 | 1216.5563 | 1285.0164 |
| | H | 1.693843 | -1.298165 | -0.017787 | 1318.2931 | 1409.2503 | 1479.2213 |
| | H | 0.321928 | 0.051047 | -3.857686 | 1516.2692 | 1636.0176 | 1668.3928 |
| | C | -2.093947 | 1.518756 | -0.24495 | 1811.6907 | 3203.874 | 3218.5981 |
| | O | -2.632641 | 2.368766 | -0.91246 | 3231.3623 | 3235.9669 | 3808.0331 |
| | O | -2.490375 | 1.189407 | 0.975656 | | | |
| | H | -3.218346 | 1.770834 | 1.241666 | | | |
| TS (-0.006) | C | -0.040760 | -0.018136 | -0.040498 | -330.9343 | 38.5399 | 55.8882 |
| | N | -0.017547 | -0.056162 | 1.892426 | 71.2887 | 82.8226 | 110.832 |
| | C | 2.435187 | -0.008685 | -1.466716 | 154.0835 | 166.1783 | 186.7002 |
| | C | 1.774474 | -1.188824 | -1.200876 | 220.2746 | 234.3533 | 253.1055 |
| | C | 1.824487 | 1.191104 | -1.056549 | 299.0025 | 321.6449 | 351.5558 |
| | H | 2.192050 | -2.142304 | -1.504831 | 410.8097 | 438.966 | 446.5599 |
| | H | 2.300412 | 2.142147 | -1.272315 | 513.9967 | 540.7327 | 587.7827 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|----------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | C | 0.547649 | -1.228754 | -0.521505 | 628.1687 | 647.5854 | 657.9581 |
| | C | 0.617717 | 1.200687 | -0.402989 | 727.1939 | 740.4257 | 755.548 |
| | H | 0.143056 | 2.13509 | -0.128426 | 788.325 | 818.4503 | 849.2238 |
| | Cl | -1.861070 | 0.118268 | -0.125703 | 883.3825 | 911.6031 | 980.754 |
| | C | 1.348652 | -0.271242 | 2.384706 | 987.9704 | 1003.7807 | 1046.0562 |
| | H | 1.631936 | -1.292333 | 2.115491 | 1054.2438 | 1056.2023 | 1073.5804 |
| | H | 2.000035 | 0.41133 | 1.828239 | 1096.7386 | 1110.0539 | 1138.175 |
| | C | 1.499693 | -0.046783 | 3.886195 | 1164.8204 | 1179.8506 | 1207.4141 |
| | H | 0.829316 | -0.722467 | 4.424779 | 1235.1887 | 1274.8059 | 1326.0292 |
| | H | 1.18538 | 0.973241 | 4.12888 | 1327.317 | 1342.7308 | 1382.8906 |
| | C | 2.940679 | -0.267125 | 4.338839 | 1392.9876 | 1406.5522 | 1418.2289 |
| | H | 3.264486 | -1.289791 | 4.132236 | 1452.0865 | 1487.4013 | 1496.5814 |
| | H | 3.621124 | 0.416446 | 3.824842 | 1497.6965 | 1502.2114 | 1512.6811 |
| | H | 3.040582 | -0.095988 | 5.410502 | 1582.8755 | 1632.0458 | 1659.566 |
| | H | -0.393365 | 0.838641 | 2.205229 | 1786.592 | 3057.6273 | 3063.242 |
| | H | -0.653908 | -0.793492 | 2.192281 | 3067.204 | 3096.9214 | 3119.6752 |
| | H | 3.393302 | -0.004433 | -1.968721 | 3134.6807 | 3156.5487 | 3192.2412 |
| | C | -0.015859 | -2.559802 | -0.260372 | 3208.9609 | 3216.1111 | 3234.0001 |
| | O | 0.248761 | -3.564896 | -0.883579 | 3485.9982 | 3577.3854 | 3825.1358 |
| | O | -0.845421 | -2.590648 | 0.803163 | | | |
| | H | -1.149007 | -3.501214 | 0.924093 | | | |
| 2-chlorobenzoic acid (-0.010) | C | 0.285919 | 0.104423 | -2.768842 | 42.3411 | 116.2489 | 207.62 |
| | C | -0.781384 | 0.733736 | -2.151527 | 216.2502 | 305.4914 | 349.4344 |
| | C | 1.168887 | -0.650025 | -1.998087 | 425.7148 | 469.0603 | 498.4277 |
| | H | -1.488348 | 1.326002 | -2.719348 | 546.7104 | 607.7442 | 639.1325 |
| | H | 2.015929 | -1.148583 | -2.455272 | 704.5401 | 717.1392 | 755.4464 |
| | C | -0.992001 | 0.638194 | -0.771833 | 805.0514 | 819.6876 | 890.7204 |
| | C | 0.970349 | -0.772808 | -0.633055 | 980.2176 | 999.1081 | 1073.0864 |
| | H | 1.643766 | -1.363012 | -0.024624 | 1080.7429 | 1153.0515 | 1171.1858 |
| | H | 0.433086 | 0.20505 | -3.838368 | 1176.9593 | 1207.8045 | 1283.6919 |
| | C | -2.18289 | 1.399997 | -0.260172 | 1319.6709 | 1414.9692 | 1479.5451 |
| | O | -3.084434 | 1.738568 | -0.992908 | 1515.0677 | 1632.1453 | 1668.325 |
| | O | -2.120668 | 1.691258 | 1.023463 | 1801.2377 | 3190.4386 | 3210.1268 |
| | H | -2.919207 | 2.163733 | 1.305467 | 3225.7199 | 3232.9115 | 3794.3682 |
| Propylamine (-0.010) | N | -0.00482 | -0.000104 | -0.01292 | 129.4283 | 228.8163 | 272.3019 |
| | C | 0.013743 | -3.6E-05 | 2.516919 | 291.6848 | 451.8961 | 747.1015 |
| | C | 0.815043 | -1.8E-05 | 1.2175 | 867.8055 | 881.4374 | 975.3154 |
| | H | 1.468285 | -0.877267 | 1.187048 | 1038.5763 | 1051.8815 | 1091.9908 |
| | H | 1.468198 | 0.877294 | 1.187008 | 1154.7941 | 1240.0205 | 1325.8327 |
| | H | -0.640964 | -0.879062 | 2.528736 | 1327.1552 | 1387.0294 | 1398.1833 |
| | H | -0.641019 | 0.87895 | 2.528725 | 1419.6731 | 1481.8634 | 1496.1188 |
| | C | 0.902809 | 0 | 3.757556 | 1499.8651 | 1509.6193 | 1654.1961 |
| | H | 1.544042 | -0.884085 | 3.783213 | 3038.5294 | 3059.9182 | 3067.0595 |
| | H | 1.544027 | 0.884098 | 3.783174 | 3071.2272 | 3104.8405 | 3134.9538 |
| | H | 0.305946 | 1.5E-05 | 4.66948 | 3156.8252 | 3501.4187 | 3571.9859 |
| | H | -0.625845 | 0.804465 | 0.032677 | | | |
| | H | -0.625489 | -0.804954 | 0.032548 | | | |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|----------------------|---------------------------|-----------|-----------|------------------------------|-----------|-----------|-----------|
| TS (-0.010) | C | -0.063916 | -0.02867 | -0.086097 | -287.7244 | 37.4258 | 57.3982 |
| | N | -0.021639 | -0.079076 | 1.925313 | 73.1774 | 83.8518 | 110.9628 |
| | C | 2.44604 | -0.026805 | -1.436158 | 154.6093 | 165.6928 | 180.3178 |
| | C | 1.764611 | -1.205339 | -1.207069 | 213.6688 | 226.9266 | 245.2123 |
| | C | 1.838293 | 1.174097 | -1.027969 | 295.7894 | 321.6621 | 350.7095 |
| | H | 2.187253 | -2.159488 | -1.502311 | 415.7276 | 434.8967 | 442.0775 |
| | H | 2.338304 | 2.121557 | -1.200887 | 507.288 | 543.0989 | 593.5069 |
| | C | 0.51734 | -1.2372 | -0.569628 | 607.3615 | 637.1999 | 654.5725 |
| | C | 0.608519 | 1.186711 | -0.41561 | 726.8322 | 740.4463 | 753.9504 |
| | H | 0.141001 | 2.1204 | -0.127219 | 791.982 | 818.5252 | 852.8276 |
| | Cl | -1.8674 | 0.109087 | -0.139672 | 881.6723 | 908.4643 | 979.0832 |
| | C | 1.351529 | -0.275903 | 2.407619 | 998.9238 | 1005.358 | 1042.9796 |
| | H | 1.642798 | -1.299061 | 2.152822 | 1053.3206 | 1056.3689 | 1060.1232 |
| | H | 1.993651 | 0.404836 | 1.836776 | 1092.6205 | 1112.9518 | 1148.7253 |
| | C | 1.520098 | -0.02496 | 3.904556 | 1159.3066 | 1179.9336 | 1206.0291 |
| | H | 0.868453 | -0.701716 | 4.463772 | 1234.6202 | 1274.6172 | 1327.4385 |
| | H | 1.190864 | 0.993356 | 4.134399 | 1329.4266 | 1340.569 | 1382.465 |
| | C | 2.969801 | -0.211768 | 4.343477 | 1396.9607 | 1401.3215 | 1418.1377 |
| | H | 3.309552 | -1.233012 | 4.155944 | 1455.5696 | 1485.9578 | 1495.6743 |
| | H | 3.632862 | 0.475219 | 3.810716 | 1497.6536 | 1501.2999 | 1511.8295 |
| | H | 3.077098 | -0.018436 | 5.410444 | 1586.7071 | 1635.2038 | 1656.6359 |
| H | -0.400749 | 0.809752 | 2.251887 | 1776.9368 | 3051.3373 | 3060.3765 | |
| H | -0.644824 | -0.818223 | 2.246836 | 3066.6746 | 3097.0238 | 3114.4935 | |
| H | 3.429252 | -0.029303 | -1.888206 | 3133.2512 | 3159.56 | 3191.349 | |
| C | -0.076474 | -2.567595 | -0.347624 | 3206.7124 | 3218.3546 | 3228.0203 | |
| O | 0.137924 | -3.54223 | -1.039126 | 3486.0091 | 3576.9912 | 3819.1692 | |
| O | -0.857707 | -2.622296 | 0.739461 | | | | |
| H | -1.170494 | -3.530059 | 0.862375 | | | | |
| | Solvent (Ethanol) | | | | | | |
| 2-chlorobenzoic acid | C | 2.163552 | -1.449974 | 0.091666 | 46.416 | 116.1585 | 197.3188 |
| | C | 0.790949 | -1.637367 | 0.042053 | 205.3854 | 298.2694 | 346.1907 |
| | C | 2.679258 | -0.157767 | 0.082147 | 416.7724 | 458.2838 | 487.2204 |
| | H | 0.368987 | -2.634713 | 0.043244 | 552.3225 | 581.5877 | 638.8215 |
| | H | 3.749344 | 0.005584 | 0.116827 | 698.8204 | 720.1985 | 771.9734 |
| | C | -0.087494 | -0.550334 | 0.00255 | 801.0389 | 819.8635 | 905.837 |
| | C | 1.825346 | 0.935733 | 0.015493 | 999.9536 | 1030.8721 | 1061.6843 |
| | H | 2.218139 | 1.943682 | -0.016051 | 1073.3607 | 1152.4141 | 1164.189 |
| | C | 0.44909 | 0.740665 | -0.019829 | 1183.2474 | 1225.2175 | 1291.5522 |
| | Cl | -0.547089 | 2.164172 | -0.170422 | 1314.4987 | 1396.3494 | 1479.0545 |
| | H | 2.825714 | -2.305052 | 0.135168 | 1519.3602 | 1639.0232 | 1665.7968 |
| | C | -1.54275 | -0.892998 | -0.017746 | 1809.8833 | 3216.9898 | 3224.7066 |
| | O | -1.975252 | -1.881929 | -0.554735 | 3233.7423 | 3239.308 | 3803.1071 |
| | O | -2.31219 | -0.040819 | 0.659842 | | | |
| H | -3.229839 | -0.346195 | 0.599126 | | | | |
| Propylamine | C | -0.587659 | -0.513628 | -0.000084 | 127.0109 | 227.5014 | 268.5939 |
| | H | -0.479973 | -1.159384 | 0.877070 | 271.6368 | 449.2291 | 742.5985 |
| | H | -0.479852 | -1.159254 | -0.877323 | 860.1096 | 864.9081 | 933.6051 |
| | C | 0.529940 | 0.528837 | 0.000054 | 1035.9141 | 1050.4525 | 1106.398 |
| | H | 0.414889 | 1.171750 | 0.879420 | 1147.7464 | 1238.887 | 1323.8901 |
| | H | 0.414936 | 1.171903 | -0.879212 | 1326.4711 | 1387.1345 | 1403.1632 |
| | C | 1.914764 | -0.114478 | 0.000016 | 1404.8372 | 1475.6886 | 1492.1663 |
| | H | 2.050677 | -0.744416 | 0.883088 | 1494.8556 | 1505.1808 | 1649.6993 |
| | H | 2.050632 | -0.744374 | -0.883093 | 3044.1316 | 3054.1257 | 3056.4575 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|----------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | H | 2.705287 | 0.637980 | 0.000013 | 3075.6001 | 3100.1893 | 3123.5196 |
| | N | -1.950895 | 0.025125 | -0.000091 | 3134.8678 | 3521.2922 | 3597.4779 |
| | H | -2.081029 | 0.623465 | -0.810740 | | | |
| | H | -2.081577 | 0.622061 | 0.811500 | | | |
| TS | C | -1.041475 | 2.353410 | -1.353877 | -374.2197 | 38.1752 | 56.7971 |
| | C | -1.209127 | 1.018417 | -1.639094 | 67.6607 | 80.0929 | 109.5154 |
| | C | -0.757894 | 2.710399 | -0.020088 | 147.2925 | 167.1872 | 189.2015 |
| | H | -1.445450 | 0.692155 | -2.645723 | 220.9637 | 233.4462 | 252.4831 |
| | H | -0.656250 | 3.756519 | 0.248707 | 297.7131 | 314.5817 | 352.1754 |
| | C | -1.084108 | 0.013520 | -0.661220 | 406.7267 | 439.7117 | 449.1096 |
| | C | -0.639480 | 1.769226 | 0.970070 | 513.2789 | 527.8201 | 561.3599 |
| | H | -0.465418 | 2.064882 | 1.997717 | 626.3829 | 640.3259 | 676.5199 |
| | C | -0.741763 | 0.368685 | 0.681542 | 724.758 | 742.4193 | 753.6405 |
| | Cl | -1.583846 | -0.549573 | 2.040944 | 785.1043 | 816.3624 | 846.9426 |
| | C | 1.931449 | 0.031138 | 0.063464 | 882.4925 | 909.7534 | 965.1289 |
| | H | 1.600502 | -0.402007 | -0.884110 | 991.5536 | 1010.9789 | 1045.8349 |
| | H | 1.868322 | 1.119972 | -0.029223 | 1053.5933 | 1054.1023 | 1075.0344 |
| | C | 3.359408 | -0.402107 | 0.376585 | 1101.3337 | 1107.8587 | 1126.8487 |
| | H | 3.388176 | -1.4897 | 0.491632 | 1166.4838 | 1177.715 | 1202.3459 |
| | H | 3.66597 | 0.030624 | 1.333613 | 1234.7093 | 1270.1348 | 1321.856 |
| | C | 4.320366 | 0.034634 | -0.72664 | 1328.0251 | 1337.9508 | 1385.4489 |
| | H | 4.039104 | -0.407618 | -1.685342 | 1391.0647 | 1410.0208 | 1411.5726 |
| | H | 4.312873 | 1.121208 | -0.841519 | 1448.2122 | 1480.3961 | 1490.8027 |
| | H | 5.34183 | -0.273512 | -0.499699 | 1494.5454 | 1494.7402 | 1509.1281 |
| | N | 0.957838 | -0.369983 | 1.082507 | 1578.5119 | 1620.6907 | 1658.0883 |
| | H | 1.205796 | -0.025318 | 2.009185 | 1763.5993 | 3058.3304 | 3061.4436 |
| | H | 0.841452 | -1.381371 | 1.126863 | 3070.0855 | 3095.0403 | 3122.1668 |
| | H | -1.141735 | 3.10742 | -2.122471 | 3133.3717 | 3143.2747 | 3196.8064 |
| | C | -1.215009 | -1.370052 | -1.119372 | 3211.4157 | 3217.856 | 3236.6191 |
| | O | -1.697973 | -1.720537 | -2.175735 | 3488.3326 | 3580.901 | 3820.3237 |
| | O | -0.683807 | -2.27802 | -0.267776 | | | |
| | H | -0.814613 | -3.15581 | -0.653355 | | | |
| 2-chlorobenzoic acid (-0.006) | C | -0.031421 | -0.030432 | 0.004454 | 31.5795 | 114.9101 | 207.0533 |
| | Cl | -0.052979 | -0.096028 | 1.732071 | 214.2204 | 304.2312 | 347.3079 |
| | C | 0.221858 | 0.024285 | -2.777953 | 425.6986 | 466.7573 | 497.2586 |
| | C | -0.733108 | 0.800446 | -2.143327 | 546.6312 | 599.3384 | 638.5612 |
| | C | 1.057081 | -0.788423 | -2.014422 | 704.309 | 714.9675 | 760.5515 |
| | H | -1.391115 | 1.446411 | -2.710967 | 803.954 | 820.5113 | 899.2935 |
| | H | 1.813744 | -1.402708 | -2.487894 | 990.577 | 1014.5143 | 1071.2841 |
| | C | -0.887235 | 0.782365 | -0.752509 | 1075.7716 | 1150.63 | 1168.0707 |
| | C | 0.934668 | -0.810104 | -0.633885 | 1175.7687 | 1213.6882 | 1283.5531 |
| | H | 1.589033 | -1.425318 | -0.029662 | 1316.654 | 1408.7517 | 1477.9345 |
| | H | 0.317420 | 0.054217 | -3.856670 | 1514.5195 | 1633.0495 | 1666.0144 |
| | C | -1.976755 | 1.668306 | -0.222657 | 1786.1779 | 3204.6592 | 3218.7921 |
| | O | -2.412972 | 2.598738 | -0.861640 | 3229.3892 | 3233.8976 | 3788.1927 |
| | O | -2.437285 | 1.31353 | 0.963364 | | | |
| | H | -3.110177 | 1.946157 | 1.260069 | | | |
| Propylamine (-0.006) | N | -0.003439 | -0.000116 | -0.007953 | 126.3406 | 226.0893 | 271.6115 |
| | C | 0.008753 | -0.000029 | 2.520528 | 278.926 | 450.3261 | 746.1863 |
| | C | 0.811779 | -0.000010 | 1.221901 | 865.5203 | 879.7791 | 969.5031 |
| | H | 1.464973 | -0.877707 | 1.195924 | 1039.0906 | 1051.8517 | 1094.861 |
| | H | 1.464853 | 0.877774 | 1.195873 | 1153.9065 | 1239.3259 | 1325.4868 |
| | H | -0.644857 | -0.879341 | 2.532066 | 1326.2403 | 1386.0903 | 1399.5211 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|----------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-----------|-----------|
| | H | -0.644937 | 0.879225 | 2.532042 | 1412.149 | 1475.3267 | 1492.3672 |
| | C | 0.902086 | 0.000031 | 3.758021 | 1493.5309 | 1506.1038 | 1646.3298 |
| | H | 1.544053 | -0.883965 | 3.778299 | 3041.8164 | 3056.3349 | 3062.7922 |
| | H | 1.544003 | 0.884064 | 3.778257 | 3074.3015 | 3101.8667 | 3129.9542 |
| | H | 0.309230 | 0.000035 | 4.672896 | 3150.8772 | 3504.4785 | 3574.7062 |
| | H | -0.623775 | 0.805365 | 0.026173 | | | |
| | H | -0.623255 | -0.806003 | 0.025978 | | | |
| TS (-0.006) | C | -0.040131 | -0.017647 | -0.062128 | -317.0321 | 31.0971 | 47.7881 |
| | N | -0.023068 | -0.053992 | 1.942629 | 65.5514 | 79.6646 | 107.3503 |
| | C | 2.489163 | -0.025008 | -1.374465 | 148.7898 | 165.0706 | 178.5262 |
| | C | 1.808271 | -1.201985 | -1.142777 | 213.5548 | 225.2467 | 245.1279 |
| | C | 1.872249 | 1.180051 | -0.989080 | 295.2041 | 318.7725 | 349.9612 |
| | H | 2.240983 | -2.156578 | -1.421310 | 413.6627 | 434.5924 | 442.9219 |
| | H | 2.370461 | 2.126528 | -1.170809 | 506.7602 | 540.0747 | 582.2144 |
| | C | 0.548364 | -1.230866 | -0.524783 | 613.9895 | 637.2528 | 650.9116 |
| | C | 0.634267 | 1.196504 | -0.393856 | 724.8764 | 740.0633 | 752.5974 |
| | H | 0.162106 | 2.132598 | -0.121283 | 790.8446 | 817.4278 | 854.4912 |
| | Cl | -1.845938 | 0.123989 | -0.143290 | 878.9288 | 907.9856 | 982.7909 |
| | C | 1.341102 | -0.298728 | 2.421669 | 996.0804 | 1007.2764 | 1043.2626 |
| | H | 1.599801 | -1.328089 | 2.156880 | 1052.3491 | 1055.0225 | 1058.1658 |
| | H | 2.004432 | 0.368489 | 1.859653 | 1097.4927 | 1110.4525 | 1145.6538 |
| | C | 1.517596 | -0.072539 | 3.92075 | 1160.5507 | 1177.225 | 1202.1016 |
| | H | 0.840538 | -0.73315 | 4.468749 | 1234.7271 | 1271.8004 | 1323.7764 |
| | H | 1.226695 | 0.954202 | 4.16264 | 1328.1068 | 1338.8081 | 1383.7047 |
| | C | 2.959631 | -0.320687 | 4.354512 | 1396.1979 | 1403.6581 | 1411.8123 |
| | H | 3.259291 | -1.35095 | 4.147856 | 1453.0209 | 1478.9869 | 1492.0338 |
| | H | 3.646617 | 0.348121 | 3.829126 | 1493.9015 | 1496.2003 | 1508.1254 |
| | H | 3.076893 | -0.147761 | 5.424204 | 1584.1539 | 1628.7729 | 1653.8103 |
| | H | -0.367891 | 0.853621 | 2.254389 | 1751.7895 | 3051.9974 | 3058.895 |
| | H | -0.672635 | -0.766654 | 2.27126 | 3067.0107 | 3096.6235 | 3113.5524 |
| | H | 3.474779 | -0.028766 | -1.820805 | 3130.5147 | 3153.8168 | 3195.8898 |
| | C | -0.039837 | -2.558687 | -0.285234 | 3207.3016 | 3218.3147 | 3230.5046 |
| | O | 0.21428 | -3.552829 | -0.938185 | 3488.1175 | 3578.6759 | 3810.2353 |
| | O | -0.866385 | -2.592199 | 0.766355 | | | |
| | H | -1.173355 | -3.500294 | 0.90514 | | | |
| 2-chlorobenzoic acid (-0.010) | C | -0.134330 | -0.147369 | -0.010496 | 44.645 | 113.4604 | 204.0678 |
| | Cl | -0.347912 | -0.430780 | 1.672557 | 213.8129 | 306.246 | 348.9478 |
| | C | 0.297251 | 0.114701 | -2.764822 | 423.1814 | 467.6779 | 496.2636 |
| | C | -0.726588 | 0.809812 | -2.142797 | 551.1264 | 606.9154 | 636.9181 |
| | C | 1.115972 | -0.717628 | -2.001776 | 703.5278 | 717.31 | 750.7641 |
| | H | -1.378538 | 1.466417 | -2.706056 | 804.2358 | 819.2577 | 890.6608 |
| | H | 1.929313 | -1.267445 | -2.461281 | 975.1519 | 1001.8956 | 1069.1139 |
| | C | -0.954946 | 0.703262 | -0.766678 | 1079.799 | 1148.6636 | 1170.0842 |
| | C | 0.897399 | -0.851338 | -0.640460 | 1174.109 | 1200.6776 | 1281.0182 |
| | H | 1.522030 | -1.499799 | -0.039115 | 1318.4146 | 1416.6127 | 1477.4549 |
| | H | 0.462783 | 0.226498 | -3.830751 | 1512.914 | 1628.2282 | 1665.0258 |
| | C | -2.089383 | 1.538786 | -0.241225 | 1772.6674 | 3188.917 | 3210.9744 |
| | O | -2.995123 | 1.900746 | -0.962865 | 3222.0851 | 3230.036 | 3775.0078 |
| | O | -1.966817 | 1.862299 | 1.024625 | | | |
| | H | -2.730356 | 2.373281 | 1.339511 | | | |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|-------------------------|---------------------------|-----------|-----------|------------------------------|-----------|-----------|-----------|
| Propylamine (-0.010) | N | -0.006720 | -0.000129 | -0.012953 | 128.318 | 228.8724 | 273.6368 |
| | C | 0.014524 | -3.6E-05 | 2.514036 | 292.5639 | 451.4803 | 746.7441 |
| | C | 0.819844 | -8E-06 | 1.217885 | 868.2113 | 884.7942 | 987.0399 |
| | H | 1.47128 | -0.878631 | 1.187814 | 1039.4537 | 1051.4847 | 1086.5669 |
| | H | 1.471146 | 0.878712 | 1.187758 | 1159.8982 | 1238.6285 | 1325.4618 |
| | H | -0.639182 | -0.879603 | 2.523159 | 1326.1892 | 1384.865 | 1395.1685 |
| | H | -0.639281 | 0.879459 | 2.523136 | 1415.8162 | 1474.3021 | 1491.7955 |
| | C | 0.899851 | 2.9E-05 | 3.757313 | 1493.3977 | 1505.9708 | 1644.9858 |
| | H | 1.540111 | -0.884659 | 3.785721 | 3040.0101 | 3057.9102 | 3066.1861 |
| | H | 1.540046 | 0.884764 | 3.785678 | 3073.2792 | 3103.8274 | 3134.1126 |
| | H | 0.298271 | 2.8E-05 | 4.66607 | 3157.0084 | 3497.0403 | 3563.5401 |
| | H | -0.630431 | 0.802263 | 0.047261 | | | |
| H | -0.629993 | -0.80287 | 0.047126 | | | | |
| TS (-0.010) | C | -0.070678 | -0.030188 | -0.119187 | -270.6497 | 23.8691 | 53.7577 |
| | N | -0.030329 | -0.095789 | 1.988441 | 63.5183 | 74.7202 | 103.4347 |
| | C | 2.496424 | -0.051757 | -1.331381 | 147.3866 | 160.2632 | 169.5613 |
| | C | 1.788034 | -1.224951 | -1.153236 | 197.4195 | 210.0002 | 240.967 |
| | C | 1.888517 | 1.154836 | -0.941602 | 292.1984 | 311.1768 | 349.619 |
| | H | 2.22208 | -2.181297 | -1.424553 | 417.4779 | 426.6167 | 437.3431 |
| | H | 2.4178 | 2.094043 | -1.062908 | 495.0842 | 527.7553 | 565.1251 |
| | C | 0.505848 | -1.240786 | -0.587652 | 591.7075 | 633.2652 | 658.2048 |
| | C | 0.624729 | 1.17836 | -0.397721 | 722.5414 | 740.724 | 750.7887 |
| | H | 0.163654 | 2.113193 | -0.102906 | 793.9315 | 816.1723 | 857.7078 |
| | Cl | -1.858941 | 0.116545 | -0.155668 | 876.7181 | 904.3371 | 975.6144 |
| | C | 1.348018 | -0.297392 | 2.44929 | 1005.1657 | 1014.2171 | 1034.5427 |
| | H | 1.634961 | -1.321289 | 2.189244 | 1040.2057 | 1054.5355 | 1057.3598 |
| | H | 1.98562 | 0.385818 | 1.874962 | 1093.6419 | 1115.3314 | 1154.562 |
| | C | 1.547807 | -0.052271 | 3.943977 | 1155.0992 | 1176.3933 | 1197.3685 |
| | H | 0.910604 | -0.734225 | 4.512574 | 1234.2615 | 1271.5829 | 1323.4581 |
| | H | 1.219035 | 0.963431 | 4.184047 | 1327.8721 | 1337.3185 | 1382.1216 |
| | C | 3.007144 | -0.235185 | 4.350432 | 1396.9897 | 1402.9432 | 1411.5269 |
| | H | 3.346435 | -1.254765 | 4.151341 | 1456.4568 | 1477.1825 | 1489.6657 |
| | H | 3.65564 | 0.458134 | 3.806902 | 1494.6429 | 1495.6682 | 1506.7496 |
| | H | 3.136298 | -0.046327 | 5.41583 | 1589.0647 | 1629.896 | 1649.5934 |
| | H | -0.394919 | 0.795285 | 2.325477 | 1739.9808 | 3040.5623 | 3055.0096 |
| | H | -0.648222 | -0.825642 | 2.339597 | 3069.1086 | 3089.6276 | 3110.4224 |
| | H | 3.508348 | -0.06618 | -1.715547 | 3129.4795 | 3157.2395 | 3193.6988 |
| | C | -0.121632 | -2.565566 | -0.400839 | 3203.4533 | 3219.8072 | 3226.1256 |
| | O | 0.062214 | -3.513392 | -1.145072 | 3484.3488 | 3571.6946 | 3800.0616 |
| | O | -0.880794 | -2.636098 | 0.685796 | | | |
| H | -1.205413 | -3.53985 | 0.818169 | | | | |
| | Solvent (Water) | | | | | | |
| 2-chlorobenzoic acid | C | 2.163938 | -1.449565 | 0.092269 | 46.7075 | 116.13 | 197.0149 |
| | C | 0.791318 | -1.637374 | 0.042679 | 205.1848 | 298.3016 | 346.2623 |
| | C | 2.679389 | -0.157233 | 0.082111 | 416.5543 | 458.095 | 487.0756 |
| | H | 0.369875 | -2.634959 | 0.044772 | 552.5247 | 581.493 | 638.6543 |
| | H | 3.74943 | 0.006354 | 0.116647 | 698.5309 | 720.225 | 771.8155 |
| | C | -0.087297 | -0.550479 | 0.002673 | 800.9298 | 819.6831 | 905.9135 |
| | C | 1.825236 | 0.936162 | 0.015081 | 1000.1167 | 1031.1749 | 1061.2957 |
| | H | 2.217954 | 1.944135 | -0.016925 | 1073.2373 | 1152.2648 | 1164.0049 |
| | C | 0.449097 | 0.740578 | -0.020008 | 1183.1303 | 1224.9737 | 1291.6056 |
| | Cl | -0.547971 | 2.163686 | -0.170913 | 1314.2798 | 1396.0823 | 1478.8471 |
| | H | 2.826294 | -2.304459 | 0.136329 | 1519.2335 | 1638.8291 | 1665.537 |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|----------------------------------|---------------------------|-----------|-----------|-------------------------------|-----------|-------------|-------------|
| | C | -1.542589 | -0.892723 | -0.017933 | 1808.1147 | 3217.1876 | 3224.717 |
| | O | -1.975735 | -1.879083 | -0.559405 | 3233.7423 | 3239.3419 | 3801.8661 |
| | O | -2.310955 | -0.043667 | 0.664362 | | | |
| | H | -3.229078 | -0.34793 | 0.603806 | | | |
| Propylamine | C | -0.587530 | -0.513982 | -0.000085 | 127.3859 | 227.7186 | 268.8988 |
| | H | -0.479780 | -1.159550 | 0.877198 | 272.4717 | 449.1626 | 742.5209 |
| | H | -0.479651 | -1.159423 | -0.877450 | 860.0671 | 865.9375 | 935.0322 |
| | C | 0.529704 | 0.528756 | 0.000056 | 1036.2028 | 1050.3602 | 1105.9858 |
| | H | 0.414401 | 1.171517 | 0.879473 | 1147.9696 | 1238.846 | 1323.7344 |
| | H | 0.414446 | 1.171674 | -0.879257 | 1326.4953 | 1387.151 | 1403.137 |
| | C | 1.914642 | -0.114322 | 0.000016 | 1404.3536 | 1474.9012 | 1491.7912 |
| | H | 2.050632 | -0.744196 | 0.883130 | 1494.2551 | 1504.7932 | 1648.981 |
| | H | 2.050591 | -0.744137 | -0.883148 | 3044.266 | 3053.9916 | 3056.2445 |
| | H | 2.704960 | 0.638361 | 0.000022 | 3075.7752 | 3100.1173 | 3123.2946 |
| | N | -1.950889 | 0.025168 | -0.000095 | 3134.6817 | 3520.8496 | 3596.6911 |
| | H | -2.079852 | 0.624151 | -0.810539 | | | |
| | H | -2.080417 | 0.622711 | 0.811316 | | | |
| TS | C | -1.032046 | 2.354253 | -1.355430 | -374.5172 | 38.36 | 56.9588 |
| | C | -1.201841 | 1.019594 | -1.641073 | 67.9032 | 79.9303 | 109.5715 |
| | C | -0.753136 | 2.711054 | -0.020526 | 147.4972 | 167.4312 | 188.7997 |
| | H | -1.433770 | 0.693891 | -2.648902 | 220.8646 | 233.3667 | 252.0986 |
| | H | -0.649283 | 3.756949 | 0.248233 | 297.4907 | 314.9251 | 351.659 |
| | C | -1.084031 | 0.014695 | -0.662138 | 406.9979 | 439.2763 | 448.9783 |
| | C | -0.641675 | 1.769747 | 0.970398 | 512.6059 | 526.9887 | 560.5973 |
| | H | -0.469585 | 2.065109 | 1.998452 | 626.2073 | 640.4751 | 674.217 |
| | C | -0.745560 | 0.369640 | 0.681421 | 724.64 | 741.9418 | 753.5718 |
| | Cl | -1.589423 | -0.548163 | 2.038111 | 785.3256 | 816.2314 | 847.189 |
| | C | 1.930746 | 0.026159 | 0.065432 | 881.8959 | 909.4346 | 965.6212 |
| | H | 1.601153 | -0.412824 | -0.879958 | 991.1486 | 1011.4572 | 1045.917 |
| | H | 1.866165 | 1.114469 | -0.032886 | 1053.5742 | 1053.9682 | 1073.7102 |
| | C | 3.35947 | -0.402707 | 0.381214 | 1101.528 | 1107.7724 | 1127.1807 |
| | H | 3.390001 | -1.489586 | 0.502115 | 1166.097 | 1177.2752 | 1201.8684 |
| | H | 3.664497 | 0.035901 | 1.336021 | 1234.8772 | 1269.8316 | 1321.6825 |
| | C | 4.319987 | 0.029907 | -0.723991 | 1327.7039 | 1337.6635 | 1385.6243 |
| | H | 4.039921 | -0.418183 | -1.680359 | 1391.1899 | 1409.458 | 1411.3727 |
| | H | 4.310394 | 1.115859 | -0.844646 | 1448.2139 | 1479.5629 | 1490.4512 |
| | H | 5.34198 | -0.275007 | -0.494971 | 1494.0293 | 1494.3222 | 1508.7186 |
| | N | 0.957867 | -0.371019 | 1.086459 | 1578.3511 | 1620.5427 | 1657.6665 |
| | H | 1.206552 | -0.021778 | 2.011233 | 1760.3683 | 3058.4412 | 3061.0894 |
| | H | 0.843173 | -1.382307 | 1.135757 | 3069.5151 | 3095.2732 | 3121.7087 |
| | H | -1.126298 | 3.108246 | -2.124839 | 3133.0051 | 3142.7803 | 3197.1867 |
| | C | -1.215182 | -1.368951 | -1.12055 | 3211.3771 | 3218.1385 | 3236.4858 |
| | O | -1.695724 | -1.718018 | -2.178922 | 3488.9151 | 3581.4998 | 3819.4589 |
| | O | -0.688627 | -2.277009 | -0.267638 | | | |
| | H | -0.81536 | -3.154964 | -0.654413 | | | |
| 2-chlorobenzoic acid (-0.006) | C | -0.031048 | -0.029714 | 0.00462 | 31.4831 | 114.7324 | 206.603400 |
| | Cl | -0.051825 | -0.093568 | 1.732303 | 213.7874 | 304.250300 | 347.238300 |
| | C | 0.220658 | 0.023903 | -2.777961 | 425.2799 | 466.554300 | 497.011500 |
| | C | -0.732512 | 0.802099 | -2.142957 | 546.9452 | 596.928900 | 638.237200 |
| | C | 1.054801 | -0.790236 | -2.014676 | 704.0737 | 714.973600 | 760.272400 |
| | H | -1.389698 | 1.448904 | -2.710633 | 803.7678 | 820.366200 | 899.309100 |
| | H | 1.810025 | -1.406070 | -2.488408 | 990.4147 | 1014.812300 | 1071.042200 |

| compound | Cartesian coordinates (Å) | | | frequency(cm ⁻¹) | | | |
|-------------------------|---------------------------|-----------|-----------|------------------------------|-----------|-------------|-------------|
| | C | -0.885749 | 0.784482 | -0.752057 | 1075.687 | 1150.563900 | 1168.083000 |
| | C | 0.933242 | -0.811372 | -0.633987 | 1175.5042 | 1212.761200 | 1283.587600 |
| | H | 1.586964 | -1.427620 | -0.030108 | 1316.4677 | 1408.491 | 1477.7861 |
| | H | 0.315620 | 0.053309 | -3.856749 | 1514.4149 | 1632.8292 | 1665.7861 |
| | C | -1.973010 | 1.672346 | -0.220941 | 1784.0171 | 3204.7072 | 3218.7987 |
| | O | -2.401686 | 2.609245 | -0.855958 | 3229.1593 | 3233.7989 | 3786.5393 |
| | O | -2.440484 | 1.311399 | 0.960095 | | | |
| | H | -3.110728 | 1.945453 | 1.260087 | | | |
| Propylamine (-0.006) | N | -0.003551 | -0.000119 | -0.007946 | 126.1162 | 225.9012 | 271.636300 |
| | C | 0.008805 | -0.000030 | 2.52025 | 278.5665 | 450.140100 | 746.142600 |
| | C | 0.812196 | -0.000009 | 1.221941 | 865.3788 | 880.102000 | 970.647500 |
| | H | 1.465224 | -0.877841 | 1.196027 | 1039.1641 | 1051.714900 | 1094.346500 |
| | H | 1.465097 | 0.877916 | 1.195975 | 1154.2413 | 1239.195700 | 1325.232100 |
| | H | -0.644709 | -0.879385 | 2.531512 | 1326.0988 | 1385.843600 | 1399.210400 |
| | H | -0.644796 | 0.879262 | 2.531487 | 1411.7467 | 1474.576500 | 1491.966100 |
| | C | 0.901846 | 0.000034 | 3.757951 | 1492.9133 | 1505.767100 | 1645.422800 |
| | H | 1.543736 | -0.884016 | 3.778433 | 3042.0314 | 3056.016400 | 3062.653400 |
| | H | 1.543678 | 0.884129 | 3.778389 | 3074.518 | 3101.667500 | 3129.798000 |
| | H | 0.308609 | 0.000037 | 4.672577 | 3150.8328 | 3503.997300 | 3573.862600 |
| | H | -0.624181 | 0.805162 | 0.027452 | | | |
| | H | -0.623641 | -0.805825 | 0.027251 | | | |
| TS (-0.006) | C | -0.044309 | -0.018433 | -0.06104 | -315.3444 | 30.4006 | 44.3474 |
| | N | -0.023366 | -0.057404 | 1.951512 | 64.3377 | 78.6615 | 106.6404 |
| | C | 2.487603 | -0.019501 | -1.366514 | 148.1381 | 164.9734 | 177.5221 |
| | C | 1.808274 | -1.198205 | -1.138331 | 212.2717 | 223.6711 | 244.1868 |
| | C | 1.867788 | 1.184049 | -0.981009 | 294.4213 | 317.9837 | 349.7472 |
| | H | 2.244362 | -2.15155 | -1.415935 | 413.878 | 434.0204 | 442.5468 |
| | H | 2.365452 | 2.131514 | -1.158888 | 505.6828 | 539.1237 | 580.4755 |
| | C | 0.546435 | -1.229855 | -0.524256 | 609.9971 | 636.1424 | 651.2498 |
| | C | 0.627889 | 1.197368 | -0.389306 | 724.54 | 739.8229 | 751.8897 |
| | H | 0.154170 | 2.132059 | -0.114688 | 791.0207 | 817.2293 | 855.0161 |
| | Cl | -1.849209 | 0.118938 | -0.137231 | 878.557 | 907.5855 | 982.2659 |
| | C | 1.342306 | -0.302894 | 2.42523 | 996.8999 | 1007.9197 | 1043.245 |
| | H | 1.600657 | -1.331532 | 2.156967 | 1050.9909 | 1054.8788 | 1057.1395 |
| | H | 2.003629 | 0.366399 | 1.863197 | 1097.7948 | 1110.4097 | 1146.2851 |
| | C | 1.524515 | -0.081027 | 3.924337 | 1159.9472 | 1177.0407 | 1201.4291 |
| | H | 0.850658 | -0.744458 | 4.472788 | 1234.7178 | 1271.3139 | 1323.4026 |
| | H | 1.232955 | 0.944472 | 4.170463 | 1328.2217 | 1338.0528 | 1383.8275 |
| | C | 2.968657 | -0.328287 | 4.351481 | 1396.5316 | 1403.3678 | 1411.1185 |
| | H | 3.269048 | -1.357476 | 4.140364 | 1453.1185 | 1477.8909 | 1491.4057 |
| | H | 3.652441 | 0.343406 | 3.825502 | 1493.4923 | 1495.6556 | 1507.4334 |
| | H | 3.089932 | -0.158577 | 5.421255 | 1584.2434 | 1628.2857 | 1653.1527 |
| | H | -0.366342 | 0.850141 | 2.265482 | 1748.401 | 3051.0312 | 3058.2632 |
| | H | -0.671740 | -0.769593 | 2.283429 | 3067.0703 | 3096.2085 | 3112.8613 |
| | H | 3.475040 | -0.021024 | -1.808899 | 3129.9742 | 3153.3411 | 3196.237 |
| | C | -0.040038 | -2.559262 | -0.286956 | 3206.906 | 3218.3927 | 3230.1785 |
| | O | 0.214018 | -3.550634 | -0.944898 | 3488.2381 | 3578.693 | 3808.701 |
| | O | -0.863325 | -2.596604 | 0.765624 | | | |
| | H | -1.167383 | -3.505525 | 0.906219 | | | |

| compound | Cartesian coordinates (Å) | | | frequency(cm^{-1}) | | | |
|----------------------------------|---------------------------|------------|------------|-------------------------------|------------|-------------|-------------|
| 2-chlorobenzoic acid (-0.010) | C | -0.136353 | -0.148926 | -0.010744 | 45.6778 | 113.598300 | 203.761300 |
| | Cl | -0.352420 | -0.433712 | 1.671591 | 213.621 | 306.344400 | 348.928400 |
| | C | 0.297601 | 0.115646 | -2.764567 | 422.8766 | 467.576200 | 496.187700 |
| | C | -0.725391 | 0.812091 | -2.142358 | 551.6399 | 606.641700 | 636.774200 |
| | C | 1.114306 | -0.719048 | -2.001864 | 703.5262 | 717.420100 | 750.156300 |
| | H | -1.375151 | 1.471049 | -2.705446 | 804.1468 | 819.181700 | 890.385500 |
| | H | 1.927097 | -1.26973 | -2.461293 | 974.4055 | 1002.031400 | 1068.816200 |
| | C | -0.954801 | 0.704214 | -0.766574 | 1079.7476 | 1148.426600 | 1169.897200 |
| | C | 0.894574 | -0.853986 | -0.640774 | 1174.1116 | 1200.196300 | 1280.951300 |
| | H | 1.517852 | -1.504148 | -0.039841 | 1318.2502 | 1416.8459 | 1477.3351 |
| | H | 0.464259 | 0.22861 | -3.830215 | 1512.7018 | 1627.8747 | 1664.683 |
| | C | -2.087707 | 1.541124 | -0.239996 | 1769.9416 | 3188.7424 | 3210.9713 |
| | O | -2.996469 | 1.899485 | -0.960167 | 3221.683 | 3229.9707 | 3773.0223 |
| | O | -1.959986 | 1.869765 | 1.023483 | | | |
| H | -2.722842 | 2.380126 | 1.341434 | | | | |
| Propylamine (-0.010) | N | -0.0069130 | -0.0001330 | -0.0129500 | 128.0596 | 228.807900 | 273.632300 |
| | C | 0.0146180 | -0.0000370 | 2.5137450 | 293.0844 | 451.378200 | 746.717400 |
| | C | 0.8203050 | -0.0000070 | 1.2179020 | 868.123 | 885.041600 | 987.953200 |
| | H | 1.4715610 | -0.8787780 | 1.1878500 | 1039.5058 | 1051.483400 | 1086.070800 |
| | H | 1.4714190 | 0.8788680 | 1.1877920 | 1160.3968 | 1238.482400 | 1325.318500 |
| | H | -0.6389890 | -0.8796470 | 2.5225840 | 1325.9553 | 1384.588400 | 1394.782500 |
| | H | -0.6390950 | 0.8794950 | 2.5225600 | 1415.4575 | 1473.530900 | 1491.384300 |
| | C | 0.8996060 | 0.0000330 | 3.7572570 | 1492.8014 | 1505.641200 | 1643.998200 |
| | H | 1.5397680 | -0.8847170 | 3.7859210 | 3040.2297 | 3057.540000 | 3066.084400 |
| | H | 1.5396940 | 0.8848380 | 3.7858780 | 3073.514 | 3103.587400 | 3134.002800 |
| | H | 0.2975900 | 0.0000290 | 4.6657180 | 3157.008 | 3496.637200 | 3562.764100 |
| | H | -0.6308510 | 0.8020620 | 0.0485900 | | | |
| | H | -0.6303980 | -0.8026900 | 0.0484520 | | | |
| | TS (-0.010) | C | -0.0700710 | -0.0306400 | -0.1218930 | -269.5457 | 21.4975 |
| N | | -0.0292100 | -0.1014030 | 1.9963300 | 61.3209 | 73.5907 | 102.6099 |
| C | | 2.5019890 | -0.0619730 | -1.3204040 | 145.3906 | 159.0128 | 168.7692 |
| C | | 1.7868700 | -1.2323930 | -1.1494010 | 195.1666 | 208.3706 | 241.114 |
| C | | 1.8983750 | 1.1467360 | -0.9308000 | 291.3445 | 309.5458 | 349.4038 |
| H | | 2.2186650 | -2.1901140 | -1.4195660 | 417.1396 | 425.5744 | 436.4441 |
| H | | 2.4336840 | 2.0833180 | -1.0454910 | 493.8665 | 524.3604 | 563.0546 |
| C | | 0.5013970 | -1.2427010 | -0.5911240 | 591.261 | 632.8973 | 658.4567 |
| C | | 0.6315970 | 1.1751370 | -0.3933950 | 721.5512 | 740.5834 | 750.2297 |
| H | | 0.1746040 | 2.1112660 | -0.0963250 | 793.9456 | 815.9625 | 857.9873 |
| Cl | | -1.8565070 | 0.1226420 | -0.1547440 | 876.4386 | 904.0171 | 973.5432 |
| C | | 1.3506880 | -0.2961850 | 2.4551730 | 1005.7056 | 1014.818 | 1033.4587 |
| H | | 1.6442460 | -1.3171430 | 2.1905970 | 1040.1471 | 1054.5116 | 1057.083 |
| H | | 1.983542 | 0.393935 | 1.8838 | 1093.7388 | 1115.4282 | 1154.2593 |
| C | | 1.551355 | -0.056277 | 3.950638 | 1155.5562 | 1175.6829 | 1196.2824 |
| H | | 0.920574 | -0.745745 | 4.517241 | 1234.3038 | 1270.9302 | 1322.9091 |
| H | | 1.215175 | 0.955738 | 4.195767 | 1327.7503 | 1337.2613 | 1382.314 |
| C | | 3.012892 | -0.229553 | 4.353346 | 1396.7356 | 1403.4778 | 1410.8331 |
| H | | 3.359753 | -1.245612 | 4.149066 | 1456.3111 | 1476.143 | 1488.9989 |
| H | | 3.654766 | 0.471394 | 3.811619 | 1494.2576 | 1495.1681 | 1506.0306 |
| H | | 3.142773 | -0.044381 | 5.419312 | 1589.2974 | 1630.0221 | 1648.8331 |
| H | | -0.398022 | 0.786582 | 2.33691 | 1736.2595 | 3039.5638 | 3054.2667 |
| H | | -0.642228 | -0.835041 | 2.348143 | 3069.3218 | 3088.493 | 3109.9552 |
| H | | 3.516513 | -0.080674 | -1.697542 | 3129.0945 | 3156.885 | 3193.8483 |
| C | | -0.134867 | -2.564820 | -0.411219 | 3202.8795 | 3220.0142 | 3226.1303 |

| compound | Cartesian coordinates (Å) | frequency(cm^{-1}) |
|----------|--------------------------------|-------------------------------|
| | O 0.039395 -3.507458 -1.165144 | 3484.5308 3571.1599 3798.1097 |
| | O -0.889001 -2.637928 0.677194 | |
| | H -1.21883 -3.540201 0.80781 | |