# Supplementary information for

# A Vacuum Ultraviolet Photoionization Study on the Formation of Methanimine (CH2NH) and Ethylenediamine (NH2CH2CH2NH2) in Low Temperature Interstellar Model Ices Exposed to Ionizing Radiation

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**Table S1** Data applied to calculate the irradiation dose per molecule. \* values from CASINO simulations, $ derived values based on 15 nA, 20 min irradiation of CH3NH2.

|  |  |
| --- | --- |
| initial kinetic energy of the electrons, Einit | 5 keV |
| irradiation current, I | 20 ± 2 nA |
| total number of electrons | (1.1 ± 0.3)×1014 |
| average kinetic energy of backscattered electrons, Ebs\* | 3.1 ± 0.3 keV |
| fraction of backscattered electrons, fbs\* | 0.3 ± 0.1 |
| average kinetic energy of transmitted electrons, Etrans\*, | 2.9 ± 0.3 keV |
| fraction of transmitted electrons, ftrans\* | 0.5 |
| average penetration depth, l\* | 180 ± 80 nm |
| density of the ice, ρ | 0.85 ± 0.05 g cm-3 |
| irradiated area, A | 1.0 ± 0.1 cm2 |
| total number of molecules processed$ | (3 ± 1)×1017 |
| dose per molecule, D$ | 1.0 ± 0.1 eV |

**Table S2** Theoretical values for the molecule geometry of CNH3 and C2N2H8 isomers and their ions.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **H2CNH** | | | | **H2CNH+** | | | |
| C | 0.584348 | 0.028954 | 0.000407 | C | 0.598498 | 0.023834 | -0.000021 |
| H | -1.166258 | 0.735956 | -0.000251 | H | -1.561096 | 0.309440 | -0.000069 |
| H | 1.075482 | 1.006604 | -0.000763 | H | 1.071217 | 1.022722 | 0.000044 |
| H | 1.244023 | -0.838535 | -0.000968 | H | 1.245402 | -0.864826 | 0.000009 |
| N | -0.665619 | -0.153964 | -0.000066 | N | -0.620931 | -0.087191 | 0.000021 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **3CH3N** | | | | **3CH3N+** | | | |
| C | 0.000000 | 0.000000 | -0.542736 | C | 0.000000 | 0.000000 | -0.661067 |
| H | 0.000000 | 1.027837 | -0.935418 | H | 0.000000 | 1.076160 | -0.862293 |
| H | -0.890133 | -0.513918 | -0.935418 | H | -0.931982 | -0.538080 | -0.862293 |
| H | 0.890133 | -0.513918 | -0.935418 | H | 0.931982 | -0.538080 | -0.862293 |
| N | 0.000000 | 0.000000 | 0.866096 | N | 0.000000 | 0.000000 | 0.936183 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **CHNH2** | | | | **CHNH2+** | | | |
| C | -0.763425 | 0.191020 | -0.000052 | C | -0.708468 | 0.155030 | -0.000061 |
| H | -1.247136 | -0.803479 | 0.000169 | H | -1.572427 | -0.505327 | 0.000151 |
| N | 0.525142 | -0.024423 | 0.000051 | N | 0.527230 | -0.030424 | 0.000071 |
| H | 1.162890 | 0.760881 | 0.000002 | H | 1.183835 | 0.756126 | -0.000072 |
| H | 0.988801 | -0.932556 | -0.000216 | H | 0.948786 | -0.968009 | -0.000209 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **3CHNH2** | | | | **3CHNH2+** | | | |
| C | -0.768492 | -0.000134 | 0.172029 | C | -0.849378 | 0.000034 | 0.156575 |
| H | -1.560245 | 0.000521 | -0.576784 | H | -1.468652 | -0.000260 | -0.741014 |
| N | 0.571054 | -0.000018 | -0.107523 | N | 0.616161 | -0.000017 | 0.018755 |
| H | 1.086806 | 0.834059 | 0.148853 | H | 1.125711 | 0.875811 | -0.164974 |
| H | 1.087013 | -0.833653 | 0.148415 | H | 1.126085 | -0.875639 | -0.164752 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **CH3NHNHCH3** | | | | **CH3NHNHCH3+** | | | |
| C | -0.016087 | 1.827841 | 0.099439 | C | -0.057850 | 1.881992 | 0.132329 |
| H | 0.653402 | 2.003275 | 0.944607 | H | 0.649709 | 1.977094 | 0.954431 |
| H | 0.205281 | 2.581493 | -0.656072 | H | 0.228114 | 2.564111 | -0.663288 |
| H | -1.048326 | 1.952461 | 0.449831 | H | -1.065870 | 2.120303 | 0.477022 |
| N | 0.249943 | 0.509348 | -0.466674 | N | -0.002265 | 0.526287 | -0.399047 |
| H | -0.350222 | 0.404574 | -1.280016 | H | -0.296266 | 0.340675 | -1.350792 |
| N | -0.249943 | -0.509348 | 0.466674 | N | 0.002265 | -0.526287 | 0.399047 |
| H | 0.350222 | -0.404574 | 1.280016 | H | 0.296266 | -0.340675 | 1.350792 |
| C | 0.016087 | -1.827841 | -0.099439 | C | 0.057850 | -1.881992 | -0.132329 |
| H | 1.048326 | -1.952461 | -0.449831 | H | 1.065870 | -2.120303 | -0.477022 |
| H | -0.205281 | -2.581493 | 0.656072 | H | -0.228114 | -2.564111 | 0.663288 |
| H | -0.653402 | -2.003275 | -0.944607 | H | -0.649709 | -1.977094 | -0.954431 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **H2NCH2CH2NH2** | | | | **H2NCH2CH2NH2+** | | | |
| N | 1.467235 | -0.558223 | -0.238485 | N | 1.649073 | -0.482818 | -0.106493 |
| H | 2.352613 | -0.666632 | 0.239672 | H | 2.163214 | -0.404393 | -0.970051 |
| H | 0.922827 | -1.396268 | -0.067161 | H | 1.692992 | -1.372142 | 0.365271 |
| C | 0.725558 | 0.587047 | 0.284633 | C | 0.869475 | 0.527303 | 0.347502 |
| H | 1.237868 | 1.506806 | -0.008397 | H | 1.159132 | 1.509213 | -0.013010 |
| H | 0.648177 | 0.603502 | 1.384140 | H | 0.647637 | 0.483105 | 1.407339 |
| C | -0.681973 | 0.600997 | -0.297080 | C | -0.869467 | 0.527333 | -0.347489 |
| H | -1.175813 | 1.543276 | -0.025829 | H | -1.159102 | 1.509233 | 0.013070 |
| H | -0.603702 | 0.569982 | -1.384980 | H | -0.647638 | 0.483171 | -1.407330 |
| N | -1.419651 | -0.594061 | 0.133800 | N | -1.649103 | -0.482808 | 0.106466 |
| H | -1.724299 | -0.496049 | 1.095300 | H | -2.163045 | -0.404507 | 0.970153 |
| H | -2.252264 | -0.726897 | -0.425272 | H | -1.693030 | -1.372111 | -0.365331 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **H2NCH2NHCH3** | | | | **H2NCH2NHCH3+** | | | |
| N | -1.460052 | -0.588360 | -0.115897 | N | -1.350176 | -0.650407 | -0.007934 |
| H | -2.302382 | -0.661056 | 0.440246 | H | -1.612240 | -1.020626 | 0.893078 |
| H | -1.728228 | -0.501483 | -1.088763 | H | -2.064393 | -0.813112 | -0.699780 |
| C | -0.663079 | 0.563795 | 0.288990 | C | -0.792651 | 0.639634 | -0.008171 |
| H | -0.568907 | 0.512536 | 1.386199 | H | -1.060042 | 1.262483 | 0.862094 |
| H | -1.121452 | 1.531975 | 0.046790 | H | -1.077541 | 1.228444 | -0.888505 |
| N | 0.617793 | 0.523231 | -0.390331 | N | 0.681601 | 0.622304 | 0.007315 |
| H | 1.046401 | 1.438247 | -0.364617 | H | 1.140402 | 1.522759 | 0.134171 |
| C | 1.536167 | -0.490360 | 0.113919 | C | 1.497535 | -0.547831 | -0.033942 |
| H | 2.462071 | -0.463399 | -0.460416 | H | 2.431510 | -0.319606 | -0.547820 |
| H | 1.784731 | -0.369104 | 1.179809 | H | 1.757270 | -0.853577 | 0.992699 |
| H | 1.085060 | -1.472425 | -0.013101 | H | 0.935754 | -1.360861 | -0.488921 |
| Atom | X | Y | Z | Atom | X | Y | Z |
| **(CH3)2NNH2** | | | | **(CH3)2NNH2+** | | | |
| N | -0.328929 | 0.239419 | 0.000000 | N | -0.105641 | 0.050367 | 0.000000 |
| C | -0.328929 | -0.587433 | 1.196851 | C | -0.105641 | -0.670272 | 1.268283 |
| H | -0.345336 | 0.048620 | 2.083676 | H | -0.378963 | 0.006386 | 2.075107 |
| H | -1.232089 | -1.196438 | 1.205462 | H | -0.833915 | -1.473896 | 1.205842 |
| H | 0.552509 | -1.243562 | 1.256237 | H | 0.885488 | -1.089656 | 1.458005 |
| C | -0.328929 | -0.587433 | -1.196851 | C | -0.105641 | -0.670272 | -1.268283 |
| H | -1.232089 | -1.196438 | -1.205462 | H | -0.833915 | -1.473896 | -1.205842 |
| H | -0.345336 | 0.048620 | -2.083676 | H | -0.378963 | 0.006386 | -2.075107 |
| H | 0.552509 | -1.243562 | -1.256237 | H | 0.885488 | -1.089656 | -1.458005 |
| N | 0.937043 | 0.989579 | 0.000000 | N | 0.312886 | 1.308805 | 0.000000 |
| H | 0.870093 | 1.614486 | -0.801011 | H | 0.235876 | 1.821698 | -0.868229 |
| H | 0.870093 | 1.614486 | 0.801011 | H | 0.235876 | 1.821698 | 0.868229 |

**Table S3** Theoretical infrared frequency modes for the CNH3 and C2N2H8 isomers and their ions.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| H2CNH | | | H2CNH+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 1075.5062 | 37.0005 | ν1 | 582.8914 | 118.9476 |
| 2 | 1101.4124 | 15.5365 | ν2 | 633.3062 | 132.9916 |
| 3 | 1170.0398 | 45.5313 | ν3 | 987.4739 | 10.3758 |
| 4 | 1373.3046 | 46.9702 | ν4 | 1058.5386 | 53.2054 |
| 5 | 1492.8412 | 6.5260 | ν5 | 1341.6707 | 63.0830 |
| 6 | 1713.0952 | 21.6437 | ν6 | 1730.4488 | 0.4752 |
| 7 | 3010.4982 | 52.4169 | ν7 | 2914.2190 | 105.7087 |
| 8 | 3103.8095 | 36.8335 | ν8 | 3028.5777 | 87.9035 |
| 9 | 3425.8292 | 1.0857 | ν9 | 3507.1840 | 387.2770 |
| 3CH3N | | | 3CH3N+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 963.5507 | 0.7019 | ν1 | 466.3037 | 8.6117 |
| 2 | 963.5524 | 0.7019 | ν2 | 898.2116 | 7.7179 |
| 3 | 1053.8599 | 4.9809 | ν3 | 898.2128 | 7.7178 |
| 4 | 1379.2879 | 13.3115 | ν4 | 1320.4751 | 0.1288 |
| 5 | 1419.7884 | 9.9782 | ν5 | 1352.6705 | 13.6947 |
| 6 | 1419.7887 | 9.9775 | ν6 | 1352.672 | 13.6931 |
| 7 | 2924.4886 | 2.4306 | ν7 | 2968.3363 | 63.0607 |
| 8 | 2979.3148 | 14.2024 | ν8 | 3112.1254 | 89.7423 |
| 9 | 2979.315 | 14.2047 | ν9 | 3112.1258 | 89.7373 |
| CHNH2 | | | CHNH2+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 801.4767 | 147.4518 | ν1 | 845.2991 | 35.7408 |
| 2 | 1075.3634 | 25.535 | ν2 | 893.2671 | 182.5151 |
| 3 | 1159.0683 | 12.2723 | ν3 | 965.3992 | 42.6828 |
| 4 | 1387.5623 | 12.7364 | ν4 | 1177.4118 | 15.2562 |
| 5 | 1438.5902 | 13.3644 | ν5 | 1565.7474 | 30.102 |
| 6 | 1686.9227 | 11.4576 | ν6 | 1728.7476 | 91.2312 |
| 7 | 2913.9804 | 110.6138 | ν7 | 3172.483 | 60.0396 |
| 8 | 3369.3698 | 22.9474 | ν8 | 3337.5861 | 159.5816 |
| 9 | 3534.9723 | 15.4043 | ν9 | 3439.4942 | 216.8281 |
| 3CHNH2 | | | 3CHNH2+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 520.137 | 30.9842 | ν1 | 569.0733 | 17.2517 |
| 2 | 610.4615 | 219.6403 | ν2 | 715.1091 | 116.3377 |
| 3 | 1070.3104 | 17.7116 | ν3 | 955.8706 | 34.4621 |
| 4 | 1099.6283 | 1.1623 | ν4 | 972.5576 | 8.0127 |
| 5 | 1267.8758 | 18.2884 | ν5 | 1110.2469 | 3.7313 |
| 6 | 1625.8034 | 22.7909 | ν6 | 1555.383 | 42.3441 |
| 7 | 3063.6355 | 30.2464 | ν7 | 3104.1286 | 49.0516 |
| 8 | 3464.8578 | 3.4299 | ν8 | 3316.4336 | 80.4391 |
| 9 | 3531.5805 | 14.6469 | ν9 | 3421.6898 | 194.3654 |
| CH3NHNHCH3 | | | CH3NHNHCH3+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 49.7107 | 6.3924 | ν1 | 112.8545 | 0.0751 |
| 2 | 234.2774 | 0.9594 | ν2 | 148.8191 | 3.1889 |
| 3 | 285.3485 | 0.0000 | ν3 | 155.5647 | 0.0000 |
| 4 | 292.0175 | 5.1310 | ν4 | 294.0692 | 1.9831 |
| 5 | 474.4309 | 0.0000 | ν5 | 402.9769 | 0.0000 |
| 6 | 815.9057 | 0.0000 | ν6 | 511.8491 | 0.0000 |
| 7 | 892.8219 | 132.1914 | ν7 | 590.0594 | 168.2007 |
| 8 | 960.6316 | 0.0000 | ν8 | 922.7047 | 0.0000 |
| 9 | 1044.4290 | 25.9933 | ν9 | 1026.3576 | 14.7526 |
| 10 | 1106.7215 | 0.0000 | ν10 | 1121.8020 | 24.6704 |
| 11 | 1108.4551 | 14.1059 | ν11 | 1123.8278 | 0.0000 |
| 12 | 1151.7854 | 12.4246 | ν12 | 1128.0659 | 1.6143 |
| 13 | 1181.2046 | 0.0000 | ν13 | 1220.7657 | 0.0000 |
| 14 | 1292.2594 | 0.0000 | ν14 | 1402.7582 | 0.0000 |
| 15 | 1431.1926 | 5.1148 | ν15 | 1432.3455 | 12.6587 |
| 16 | 1446.5412 | 4.7441 | ν16 | 1464.1766 | 5.2859 |
| 17 | 1446.7211 | 0.0000 | ν17 | 1468.4634 | 0.0000 |
| 18 | 1479.2835 | 0.0000 | ν18 | 1476.7806 | 29.2365 |
| 19 | 1483.8601 | 13.7356 | ν19 | 1479.2059 | 0.0000 |
| 20 | 1515.4655 | 22.3501 | ν20 | 1500.0455 | 0.0000 |
| 21 | 1517.1866 | 0.0000 | ν21 | 1505.3241 | 65.2002 |
| 22 | 1538.4557 | 0.0000 | ν22 | 1612.1145 | 0.0000 |
| 23 | 2973.5900 | 160.9774 | ν23 | 3038.1648 | 0.0000 |
| 24 | 2976.7763 | 0.0000 | ν24 | 3038.5829 | 2.2985 |
| 25 | 3046.5231 | 78.8358 | ν25 | 3116.4385 | 0.2815 |
| 26 | 3046.6431 | 0.0000 | ν26 | 3117.2818 | 0.0000 |
| 27 | 3095.6242 | 50.5520 | ν27 | 3156.6600 | 1.2636 |
| 28 | 3095.7023 | 0.0000 | ν28 | 3157.0660 | 0.0000 |
| 29 | 3450.0833 | 0.0000 | ν29 | 3548.2904 | 0.0000 |
| 30 | 3471.0086 | 0.0657 | ν30 | 3557.5745 | 168.3875 |
| (CH3)2NNH2 | | | (CH3)2NNH2+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 164.5265 | 36.2334 | ν1 | 100.5343 | 0.0109 |
| 2 | 262.6485 | 7.0780 | ν2 | 137.5117 | 0.3196 |
| 3 | 274.4501 | 0.0136 | ν3 | 291.3740 | 11.5028 |
| 4 | 408.7494 | 4.3265 | ν4 | 404.9324 | 10.2624 |
| 5 | 436.2408 | 1.8204 | ν5 | 409.7203 | 3.1825 |
| 6 | 439.5743 | 16.7883 | ν6 | 468.9608 | 0.0372 |
| 7 | 811.4670 | 14.3654 | ν7 | 527.4746 | 191.1342 |
| 8 | 982.7986 | 20.2362 | ν8 | 798.0330 | 1.1307 |
| 9 | 1039.6479 | 14.8111 | ν9 | 1027.9332 | 13.9603 |
| 10 | 1107.2052 | 0.6997 | ν10 | 1086.7726 | 4.0227 |
| 11 | 1116.1826 | 60.2056 | ν11 | 1111.9567 | 0.9131 |
| 12 | 1132.4435 | 10.5313 | ν12 | 1137.1129 | 2.2901 |
| 13 | 1199.1632 | 4.5031 | ν13 | 1159.6141 | 3.3527 |
| 14 | 1256.8760 | 0.2674 | ν14 | 1389.1960 | 0.8233 |
| 15 | 1396.6579 | 5.0630 | ν15 | 1425.1564 | 14.3774 |
| 16 | 1433.1014 | 0.9195 | ν16 | 1448.8353 | 1.2036 |
| 17 | 1460.5832 | 2.7575 | ν17 | 1465.7927 | 14.8286 |
| 18 | 1477.4936 | 9.1040 | ν18 | 1468.5245 | 0.0053 |
| 19 | 1487.7995 | 8.9362 | ν19 | 1487.3965 | 9.4913 |
| 20 | 1497.8457 | 0.2099 | ν20 | 1488.6399 | 23.4394 |
| 21 | 1511.7046 | 11.5259 | ν21 | 1526.7873 | 14.2940 |
| 22 | 1650.6901 | 34.0909 | ν22 | 1659.5838 | 79.5095 |
| 23 | 2942.0905 | 46.2139 | ν23 | 3031.4526 | 0.3176 |
| 24 | 2950.5747 | 105.9159 | ν24 | 3035.2911 | 1.5530 |
| 25 | 3051.9818 | 43.5185 | ν25 | 3117.8989 | 0.2308 |
| 26 | 3054.6447 | 30.7283 | ν26 | 3118.8408 | 0.0931 |
| 27 | 3097.9984 | 6.0858 | ν27 | 3156.4993 | 0.0642 |
| 28 | 3103.3640 | 44.1226 | ν28 | 3161.0826 | 0.6534 |
| 29 | 3421.1784 | 1.7475 | ν29 | 3513.6341 | 121.0814 |
| 30 | 3498.3215 | 0.0350 | ν30 | 3645.6045 | 106.4104 |
| NH2CH2CH2NH2 | | | NH2CH2CH2NH2+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 179.9656 | 4.2047 | ν1 | 118.9283 | 0.4519 |
| 2 | 235.6987 | 20.7799 | ν2 | 173.5474 | 0.0577 |
| 3 | 290.2833 | 44.0429 | ν3 | 334.9658 | 0.2470 |
| 4 | 348.0012 | 22.5367 | ν4 | 375.9995 | 3.6233 |
| 5 | 504.1945 | 12.0775 | ν5 | 417.6388 | 88.9136 |
| 6 | 812.9440 | 91.1544 | ν6 | 472.3067 | 13.0408 |
| 7 | 853.7207 | 75.6127 | ν7 | 516.2050 | 260.7918 |
| 8 | 878.8733 | 79.2875 | ν8 | 518.9747 | 19.2435 |
| 9 | 927.4051 | 34.2551 | ν9 | 826.9022 | 12.9578 |
| 10 | 1007.0535 | 12.4586 | ν10 | 865.4095 | 4.4735 |
| 11 | 1050.4762 | 8.4471 | ν11 | 1030.8206 | 9.5415 |
| 12 | 1111.8972 | 5.2103 | ν12 | 1073.0899 | 0.2365 |
| 13 | 1182.9452 | 4.0095 | ν13 | 1116.1998 | 0.1456 |
| 14 | 1219.1725 | 4.7418 | ν14 | 1219.8789 | 1.0774 |
| 15 | 1325.2989 | 3.0479 | ν15 | 1282.5953 | 69.0741 |
| 16 | 1342.2669 | 2.1699 | ν16 | 1290.7199 | 7.8323 |
| 17 | 1408.0343 | 8.9275 | ν17 | 1351.8296 | 3.2982 |
| 18 | 1431.9029 | 6.5813 | ν18 | 1355.1309 | 2.5404 |
| 19 | 1498.5561 | 4.4343 | ν19 | 1498.4649 | 10.5689 |
| 20 | 1511.8609 | 3.3838 | ν20 | 1500.7886 | 3.6261 |
| 21 | 1643.5125 | 35.9144 | ν21 | 1669.0592 | 61.4084 |
| 22 | 1655.7046 | 25.0305 | ν22 | 1673.0249 | 61.3540 |
| 23 | 2913.0618 | 90.1722 | ν23 | 3094.1370 | 6.9372 |
| 24 | 2963.3322 | 84.6318 | ν24 | 3100.5815 | 0.0027 |
| 25 | 3036.8892 | 48.2593 | ν25 | 3192.4228 | 0.3734 |
| 26 | 3064.3194 | 31.7873 | ν26 | 3196.4396 | 0.1725 |
| 27 | 3487.5711 | 4.5441 | ν27 | 3555.6620 | 303.5859 |
| 28 | 3492.3403 | 0.2313 | ν28 | 3566.9258 | 70.1105 |
| 29 | 3568.3256 | 3.0076 | ν29 | 3674.4148 | 121.0612 |
| 30 | 3573.3657 | 0.9236 | ν30 | 3674.6780 | 59.1663 |
| H2NCH2NHCH3 | | | H2NCH2NHCH3+ | | |
| Normal modes | Frequency(cm-1) | IR Intensity | Normal modes | Frequency(cm-1) | IR Intensity |
| 1 | 155.5951 | 3.0447 | ν1 | 110.8234 | 9.5533 |
| 2 | 199.3598 | 3.9098 | ν2 | 136.7661 | 3.8321 |
| 3 | 256.3639 | 43.6882 | ν3 | 229.1249 | 21.1248 |
| 4 | 354.2506 | 2.7450 | ν4 | 298.3746 | 1.4209 |
| 5 | 517.6992 | 6.6231 | ν5 | 520.0678 | 99.4510 |
| 6 | 742.3573 | 133.3957 | ν6 | 627.0610 | 60.7215 |
| 7 | 832.5152 | 105.1208 | ν7 | 641.4707 | 76.2000 |
| 8 | 905.6845 | 8.3208 | ν8 | 786.4589 | 3.2459 |
| 9 | 999.4335 | 10.5407 | ν9 | 832.3506 | 14.4057 |
| 10 | 1041.1852 | 13.1506 | ν10 | 1017.4395 | 41.2582 |
| 11 | 1139.8032 | 3.4008 | ν11 | 1057.1552 | 6.1410 |
| 12 | 1169.3373 | 64.2341 | ν12 | 1120.2903 | 26.2495 |
| 13 | 1182.3384 | 10.8405 | ν13 | 1170.1044 | 9.7959 |
| 14 | 1249.0761 | 8.9192 | ν14 | 1195.4672 | 7.1864 |
| 15 | 1338.5552 | 2.4211 | ν15 | 1306.6047 | 9.4839 |
| 16 | 1426.8185 | 24.4433 | ν16 | 1367.2696 | 0.9236 |
| 17 | 1455.9869 | 13.7573 | ν17 | 1383.2562 | 31.6166 |
| 18 | 1487.4081 | 12.6813 | ν18 | 1423.0346 | 10.0826 |
| 19 | 1496.4614 | 0.8865 | ν19 | 1427.8173 | 31.8465 |
| 20 | 1517.9698 | 3.0244 | ν20 | 1461.8472 | 28.6748 |
| 21 | 1523.9726 | 6.8419 | ν21 | 1494.9044 | 12.1352 |
| 22 | 1639.8778 | 30.8845 | ν22 | 1672.7270 | 48.4770 |
| 23 | 2913.6289 | 97.5123 | ν23 | 2927.5904 | 60.8846 |
| 24 | 2933.2343 | 115.6178 | ν24 | 2945.0094 | 24.0464 |
| 25 | 2958.2492 | 91.4081 | ν25 | 3009.4568 | 4.5659 |
| 26 | 3068.2083 | 37.6601 | ν26 | 3068.4715 | 5.5108 |
| 27 | 3113.2954 | 14.8337 | ν27 | 3143.3810 | 20.4867 |
| 28 | 3494.2785 | 0.3165 | ν28 | 3494.4745 | 99.8736 |
| 29 | 3541.8180 | 0.3031 | ν29 | 3562.3324 | 83.0464 |
| 30 | 3582.3946 | 0.8282 | ν30 | 3653.6543 | 68.2966 |