$coordinates

| | | | |
|---|---|---|---|
| Sn | -0.00338637409818 | 1.06820824945472 | -7.77284448206249 |
| Sn | -7.16438632016766 | -3.41706159126987 | 2.79650784991817 |
| Sn | -5.76554024763759 | 1.26878642786784 | 6.23894577018697 |
| Ag | -6.94224037056737 | -1.66655364781631 | -2.73442141586646 |
| Ag | -2.90825971638762 | 0.03833179998310 | 1.13424351757818 |
| Ag | 3.03608406070838 | 0.73581718950320 | -3.28886040532417 |
| Ag | 0.37260916376560 | 4.49968092049969 | -0.01155652374137 |
| Ag | 4.71261021847466 | 1.57689935615043 | 1.91039126660743 |
| Ag | -5.32736398405764 | -4.81849121232036 | -6.84897330427518 |
| Sn | 0.36734754640345 | 2.33902887489954 | 5.41957925335510 |
| Sn | 2.05190304276043 | -3.05100229195282 | 0.85677470183302 |
| Sn | -5.68516822644699 | 0.49466255662119 | -7.93717055700540 |
| Sn | -1.56305525468407 | -3.27259993373849 | 5.45331653197489 |
| Ag | -4.18437888255335 | 3.35428292786187 | -3.22173075900721 |
| Ag | -1.49326377227279 | -2.57076401106425 | -3.52169213822085 |
| Sn | -4.20965819301302 | 5.89359371747155 | 2.64537825784995 |
| Ag | 0.40943150343238 | 5.85420927956560 | -5.25140731551700 |
| Sn | -8.51713848407472 | 2.23375579838934 | 0.78528411752988 |

$end

vibrational frequencies, intensities

| mode | au_amu | cm-1 | km/mol |
|---|---|---|---|
| 7 | 0.003233 | 16.6 | 0.02 |
| 8 | 0.004176 | 21.5 | 0.08 |
| 9 | 0.005187 | 26.7 | 0.05 |
| 10 | 0.006052 | 31.1 | 0.07 |
| 11 | 0.006490 | 33.4 | 0.05 |
| 12 | 0.006684 | 34.4 | 0.08 |
| 13 | 0.007138 | 36.7 | 0.04 |
| 14 | 0.007637 | 39.3 | 0.13 |
| 15 | 0.007747 | 39.8 | 0.03 |
| 16 | 0.008223 | 42.3 | 0.14 |
| 17 | 0.008860 | 45.5 | 0.04 |
| 18 | 0.009289 | 47.8 | 0.10 |
| 19 | 0.009774 | 50.2 | 0.11 |
| 20 | 0.010414 | 53.5 | 0.22 |
| 21 | 0.010622 | 54.6 | 0.09 |
| 22 | 0.011057 | 56.8 | 0.03 |
| 23 | 0.011565 | 59.4 | 0.03 |
| 24 | 0.012084 | 62.1 | 0.08 |
| 25 | 0.012220 | 62.8 | 0.03 |
| 26 | 0.012861 | 66.1 | 0.10 |
| 27 | 0.013594 | 69.9 | 0.09 |
| 28 | 0.013718 | 70.5 | 0.03 |
| 29 | 0.014106 | 72.5 | 0.06 |
| 30 | 0.014542 | 74.8 | 0.10 |
| 31 | 0.014772 | 75.9 | 0.10 |
| 32 | 0.015018 | 77.2 | 0.16 |
| 33 | 0.016466 | 84.6 | 0.17 |
| 34 | 0.016501 | 84.8 | 0.20 |
| 35 | 0.016828 | 86.5 | 0.04 |

| | | | |
|---|---|---|---|
| 36 | 0.017163 | 88.2 | 0.02 |
| 37 | 0.017767 | 91.3 | 0.28 |
| 38 | 0.018661 | 95.9 | 0.01 |
| 39 | 0.018800 | 96.6 | 0.02 |
| 40 | 0.019889 | 102.2 | 0.24 |
| 41 | 0.020538 | 105.6 | 0.02 |
| 42 | 0.020727 | 106.5 | 0.07 |
| 43 | 0.021462 | 110.3 | 0.19 |
| 44 | 0.022226 | 114.3 | 0.14 |
| 45 | 0.022652 | 116.4 | 0.09 |
| 46 | 0.022962 | 118.0 | 0.03 |
| 47 | 0.023443 | 120.5 | 0.29 |
| 48 | 0.024068 | 123.7 | 0.07 |
| 49 | 0.024424 | 125.6 | 0.46 |
| 50 | 0.025696 | 132.1 | 0.48 |
| 51 | 0.025976 | 133.5 | 0.08 |
| 52 | 0.027217 | 139.9 | 0.84 |
| 53 | 0.027490 | 141.3 | 0.32 |
| 54 | 0.028412 | 146.1 | 0.54 |

Frequencies (cm-1) and normal modes

| | 7: 16.6 | 8: 21.5 | 9: 26.7 | 10: 31.1 | 11: 33.4 | 12: 34.4 | 13: 36.7 | 14: 39.3 | 15: 39.8 |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.1043 | 0.1064 | -0.1662 | 0.3726 | 0.0780 | -0.1097 | -0.0017 | -0.1045 | 0.0080 |
| y | 0.2812 | 0.1700 | 0.2296 | -0.1158 | 0.1995 | 0.2098 | 0.0518 | 0.0599 | -0.0857 |
| z | 0.1776 | -0.0171 | -0.1143 | -0.1912 | -0.0941 | 0.1439 | -0.2400 | -0.0155 | -0.1102 |
| Sn x | 0.0537 | -0.3082 | -0.1188 | -0.1111 | 0.2981 | -0.2121 | -0.0173 | 0.0236 | -0.1139 |
| y | -0.0312 | 0.1612 | 0.0526 | -0.0260 | -0.0799 | 0.0843 | -0.0133 | -0.2295 | 0.1050 |
| z | 0.0528 | -0.0023 | 0.2499 | 0.2932 | -0.0635 | 0.2392 | 0.0482 | -0.2494 | -0.0676 |
| Sn x | -0.0503 | 0.0435 | -0.0379 | 0.0581 | -0.0160 | 0.1262 | -0.1270 | -0.3032 | 0.0472 |
| y | 0.0972 | -0.0031 | 0.2132 | 0.0433 | -0.0414 | 0.0114 | -0.0459 | -0.1981 | 0.0570 |
| z | -0.0521 | 0.0090 | -0.1168 | 0.1203 | 0.0593 | 0.2610 | 0.0958 | -0.1387 | 0.0490 |
| Ag x | 0.0371 | -0.0420 | 0.1001 | -0.0086 | -0.1417 | 0.0191 | 0.0079 | -0.1503 | -0.1094 |
| y | -0.0894 | -0.0452 | -0.3784 | -0.0300 | 0.1444 | 0.1804 | -0.2735 | 0.0488 | 0.0999 |
| z | 0.0235 | 0.0877 | 0.1908 | 0.1437 | -0.1183 | -0.0637 | 0.0903 | 0.0608 | -0.2759 |
| Ag x | 0.0209 | -0.0622 | -0.0191 | -0.1482 | 0.0350 | -0.1633 | 0.0195 | -0.0962 | -0.1092 |
| y | -0.0514 | 0.0391 | -0.0976 | -0.0889 | 0.1087 | -0.0444 | -0.0266 | 0.0450 | 0.0094 |
| z | -0.0114 | -0.0388 | -0.0136 | 0.0181 | 0.0268 | 0.0169 | 0.1589 | 0.0658 | 0.1226 |
| Ag x | 0.1848 | 0.1100 | -0.1268 | 0.2776 | -0.0986 | 0.0942 | -0.0105 | 0.2456 | -0.0814 |
| y | -0.3135 | 0.1026 | 0.1766 | 0.0866 | 0.0893 | -0.1184 | -0.0092 | -0.1133 | 0.0745 |
| z | 0.0001 | -0.0406 | -0.0669 | -0.1012 | 0.0331 | -0.0636 | -0.1367 | -0.2276 | -0.0814 |
| Ag x | 0.1137 | -0.0039 | 0.1205 | -0.0986 | 0.0613 | -0.1000 | -0.1124 | 0.1538 | 0.0110 |
| y | -0.1941 | -0.0121 | -0.0084 | -0.1631 | 0.0886 | -0.1026 | -0.0737 | -0.2034 | -0.1470 |
| z | -0.1875 | -0.0113 | 0.2344 | -0.0411 | 0.1129 | -0.1180 | -0.2033 | -0.0767 | 0.2229 |
| Ag x | 0.0592 | 0.0265 | 0.1120 | -0.0300 | -0.0611 | -0.0064 | -0.1734 | 0.1902 | 0.3247 |
| y | -0.1980 | 0.0384 | -0.2043 | -0.0048 | -0.2808 | 0.0682 | 0.0828 | 0.0874 | -0.0135 |
| z | 0.0130 | 0.0059 | -0.0384 | 0.0098 | 0.0622 | -0.1213 | -0.0184 | -0.1443 | -0.2621 |
| Ag x | 0.0227 | 0.0627 | 0.1299 | -0.1497 | -0.1600 | 0.1629 | 0.1052 | 0.0246 | 0.3197 |
| y | 0.0397 | -0.3006 | -0.0255 | 0.1041 | -0.2618 | 0.0511 | 0.0865 | -0.0458 | -0.0197 |
| z | -0.0745 | 0.3256 | -0.0932 | -0.0192 | 0.1806 | 0.0247 | -0.2095 | 0.2579 | -0.1248 |
| Sn x | 0.0332 | 0.0207 | 0.0125 | -0.0833 | -0.0015 | -0.0043 | -0.0166 | -0.0271 | 0.2950 |
| y | 0.0982 | -0.2235 | -0.0138 | 0.0638 | 0.1363 | -0.0039 | -0.0207 | 0.0600 | -0.0796 |
| z | -0.0958 | 0.0130 | -0.0632 | -0.0703 | 0.0645 | -0.1136 | 0.2036 | -0.0624 | -0.0311 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.1067 | 0.0757 | -0.0747 | -0.0956 | -0.2704 | 0.0052 | -0.1225 | -0.0020 | -0.0798 |
| y | -0.1365 | 0.0564 | -0.0526 | 0.0813 | -0.1103 | 0.0038 | 0.0662 | 0.1743 | 0.1124 |
| z | 0.1102 | -0.1032 | -0.0767 | -0.1902 | -0.1486 | 0.0662 | 0.1243 | 0.0630 | 0.1101 |
| Sn x | 0.1264 | 0.1440 | -0.1693 | 0.3031 | 0.1187 | -0.0892 | -0.0475 | -0.1133 | 0.0615 |
| y | 0.0590 | -0.3297 | -0.0054 | 0.1012 | -0.2677 | -0.0363 | 0.0435 | -0.0092 | -0.0613 |
| z | 0.0024 | 0.0831 | 0.1977 | 0.0573 | -0.1878 | -0.2299 | -0.0613 | 0.2845 | -0.2181 |
| Sn x | -0.0133 | -0.1735 | -0.0439 | 0.0444 | 0.1143 | -0.0663 | -0.0993 | -0.0538 | -0.0564 |
| y | 0.1307 | -0.2147 | 0.0533 | 0.0139 | 0.1440 | -0.0314 | 0.0102 | 0.0961 | 0.0719 |
| z | 0.1748 | -0.3217 | 0.0408 | -0.0170 | 0.1489 | -0.0292 | 0.2511 | 0.0615 | 0.1719 |
| Ag x | -0.2032 | -0.0488 | 0.1147 | -0.1189 | 0.1560 | 0.2794 | 0.1171 | 0.1270 | -0.1865 |
| y | 0.0459 | -0.0227 | -0.0728 | 0.0238 | -0.1282 | -0.1874 | -0.2576 | 0.1045 | -0.0447 |
| z | 0.0923 | -0.0345 | 0.0448 | 0.0911 | -0.1210 | -0.2659 | -0.1142 | 0.0927 | 0.0713 |
| Ag x | 0.0115 | 0.0578 | 0.0959 | 0.0144 | -0.1851 | 0.0549 | -0.0310 | -0.0294 | -0.0673 |
| y | -0.0295 | 0.1192 | 0.0553 | 0.2639 | 0.2205 | -0.0660 | 0.2407 | 0.2199 | 0.1505 |
| z | -0.0401 | -0.0486 | -0.1540 | -0.2126 | -0.1646 | 0.0913 | -0.0607 | 0.1025 | 0.1242 |
| Sn x | 0.1020 | 0.1410 | -0.0768 | -0.1338 | -0.0399 | -0.1208 | 0.2521 | 0.0462 | -0.0206 |
| y | -0.0228 | 0.0702 | 0.0556 | -0.0159 | -0.0209 | -0.1430 | -0.0202 | -0.1164 | 0.0077 |
| z | -0.1612 | 0.1256 | -0.2343 | -0.0607 | 0.0282 | -0.0921 | 0.3264 | -0.0395 | 0.0674 |
| Ag x | -0.4774 | -0.2279 | 0.1795 | 0.0746 | 0.0730 | 0.2538 | -0.0105 | 0.2433 | -0.1987 |
| y | 0.3496 | 0.1636 | 0.0345 | -0.2134 | 0.1147 | 0.2757 | 0.0304 | 0.0162 | -0.2068 |
| z | -0.0180 | 0.0135 | 0.2553 | -0.0341 | 0.1159 | 0.0015 | -0.2207 | 0.0004 | 0.2044 |
| Sn x | -0.0294 | 0.0723 | 0.0014 | -0.1757 | 0.0250 | -0.0957 | 0.2637 | -0.1413 | -0.0483 |
| y | -0.0555 | 0.2347 | -0.0361 | -0.1250 | -0.0506 | -0.1488 | 0.1192 | 0.0109 | -0.0345 |
| z | -0.0156 | -0.0333 | -0.2254 | 0.1972 | 0.0713 | 0.2294 | -0.0670 | -0.0291 | 0.0274 |

16: 42.3 17: 45.5 18: 47.8 19: 50.2 20: 53.5 21: 54.6 22: 56.8 23: 59.4 24: 62.1

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.0276 | 0.1187 | -0.2303 | -0.0569 | 0.0232 | 0.0253 | -0.0488 | -0.0046 | -0.0357 |
| y | 0.0020 | 0.1635 | 0.0163 | 0.0584 | 0.1579 | 0.1023 | 0.0169 | -0.0771 | -0.1335 |
| z | -0.2559 | -0.0849 | -0.1006 | 0.1287 | -0.1089 | -0.2003 | 0.0485 | 0.0198 | 0.3006 |
| Sn x | 0.0213 | -0.0729 | 0.0995 | 0.0070 | 0.3434 | -0.1839 | -0.1107 | 0.0358 | 0.2227 |
| y | -0.0224 | -0.0099 | 0.0423 | 0.0662 | -0.0757 | 0.1099 | 0.0344 | 0.0796 | -0.0233 |
| z | -0.0354 | -0.0304 | -0.0386 | -0.0104 | 0.0657 | -0.0231 | -0.0643 | 0.0109 | 0.1241 |
| Sn x | -0.0428 | -0.0627 | 0.0010 | 0.0107 | 0.1463 | 0.1459 | 0.1753 | -0.1939 | -0.0776 |
| y | -0.0227 | -0.0380 | 0.1124 | -0.0613 | 0.2211 | 0.0151 | -0.0572 | -0.0151 | 0.2641 |
| z | 0.1100 | -0.0514 | 0.0220 | -0.0367 | -0.0147 | -0.0833 | 0.1929 | 0.1678 | -0.0895 |
| Ag x | 0.3159 | 0.1935 | 0.1820 | 0.0281 | -0.0285 | -0.1683 | -0.1261 | 0.1981 | -0.0642 |
| y | 0.2029 | 0.0491 | 0.2346 | -0.0526 | -0.0923 | 0.2051 | -0.1283 | -0.0431 | 0.0911 |
| z | 0.0210 | 0.0283 | -0.0676 | -0.0080 | 0.0341 | -0.2142 | -0.2332 | 0.0697 | -0.2021 |
| Ag x | 0.0269 | 0.0506 | 0.0988 | -0.0782 | 0.0476 | 0.1006 | -0.0281 | 0.0351 | -0.0230 |
| y | 0.0428 | -0.1950 | -0.1404 | -0.0245 | 0.2151 | -0.3134 | -0.0196 | 0.2718 | -0.1120 |
| z | -0.0507 | -0.0833 | -0.0565 | -0.0794 | -0.0117 | 0.1068 | -0.1928 | 0.0130 | 0.0211 |
| Ag x | -0.1759 | -0.1397 | 0.1744 | 0.1364 | -0.0715 | -0.1201 | -0.0087 | 0.1996 | 0.3021 |
| y | 0.0944 | -0.1203 | 0.1224 | -0.1623 | -0.3812 | -0.2144 | -0.0807 | -0.2265 | 0.2776 |
| z | -0.0940 | -0.0108 | -0.1598 | -0.0728 | -0.0513 | -0.1376 | 0.1287 | -0.2923 | -0.0811 |
| Ag x | 0.0059 | -0.1411 | 0.0766 | -0.3404 | -0.0332 | -0.0106 | 0.1565 | 0.2443 | -0.0975 |
| y | 0.1556 | 0.0030 | -0.3581 | -0.2210 | 0.0187 | -0.0035 | 0.0226 | 0.1894 | 0.0338 |
| z | -0.0972 | 0.1104 | 0.0529 | -0.0050 | 0.0080 | 0.0428 | -0.0443 | 0.2142 | -0.0277 |
| Ag x | -0.1131 | 0.1102 | -0.0298 | -0.1849 | -0.1583 | -0.2962 | 0.1010 | -0.1188 | -0.1204 |
| y | -0.2380 | 0.2661 | 0.0143 | -0.1004 | 0.1910 | 0.1228 | 0.0901 | 0.0062 | 0.0932 |
| z | -0.1168 | -0.2944 | 0.2548 | -0.0759 | -0.1078 | -0.0531 | 0.1851 | -0.2541 | -0.1601 |
| Ag x | 0.3213 | -0.4695 | -0.1016 | 0.2274 | 0.0757 | 0.1627 | 0.0304 | -0.0123 | 0.0043 |
| y | -0.0382 | -0.0958 | -0.0093 | -0.0782 | -0.0367 | -0.0716 | -0.2398 | 0.0040 | -0.1420 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| z | 0.1673 | 0.0518 | 0.0754 | -0.0021 | -0.0066 | 0.0305 | -0.3397 | -0.1610 | -0.1172 |
| Sn x | -0.0571 | 0.0957 | -0.2175 | 0.0080 | 0.0001 | -0.1267 | -0.0786 | -0.1625 | 0.0087 |
| y | -0.0289 | -0.0395 | 0.0399 | 0.1793 | -0.2353 | 0.1175 | 0.2423 | 0.1433 | -0.3167 |
| z | -0.1064 | -0.0717 | 0.2707 | -0.0124 | 0.1817 | 0.1691 | -0.0925 | 0.1284 | -0.0089 |
| Sn x | -0.1773 | 0.0074 | 0.1027 | -0.0271 | -0.0166 | 0.1547 | -0.0964 | -0.0410 | -0.2302 |
| y | -0.1927 | 0.1108 | 0.1284 | -0.1259 | 0.0364 | -0.0879 | 0.1874 | 0.0368 | 0.0818 |
| z | 0.0971 | 0.2290 | 0.0216 | -0.1846 | 0.1655 | -0.0425 | 0.0659 | -0.1693 | -0.2052 |
| Sn x | 0.0147 | 0.1636 | -0.2428 | -0.0418 | 0.0399 | 0.0785 | -0.0850 | 0.0505 | -0.0125 |
| y | -0.0128 | -0.0203 | -0.0648 | -0.0669 | -0.0415 | 0.0200 | -0.1315 | -0.0205 | -0.0450 |
| z | 0.1360 | -0.0301 | -0.2103 | 0.0241 | -0.0048 | 0.2002 | 0.2151 | -0.0431 | 0.1139 |
| Sn x | -0.2236 | -0.0889 | -0.0826 | 0.2636 | -0.1833 | 0.2203 | -0.1903 | -0.0750 | -0.0967 |
| y | 0.0084 | 0.0731 | -0.0333 | 0.1757 | -0.2470 | -0.0728 | 0.1069 | 0.0852 | -0.1109 |
| z | 0.1058 | 0.2040 | 0.0680 | -0.0201 | -0.1064 | 0.1012 | -0.1082 | -0.2214 | 0.2172 |
| Ag x | -0.0326 | 0.0297 | -0.1322 | -0.2800 | -0.2170 | 0.2289 | -0.0131 | 0.1762 | 0.1261 |
| y | 0.2937 | 0.0392 | 0.0010 | 0.2042 | 0.1774 | -0.0454 | 0.1290 | -0.1575 | 0.0592 |
| z | 0.1107 | 0.0031 | -0.0733 | -0.1086 | -0.0588 | 0.3324 | 0.1484 | 0.0871 | 0.1686 |
| Ag x | 0.2736 | 0.1219 | 0.2489 | 0.0357 | -0.1329 | -0.0878 | -0.0837 | -0.0054 | -0.0363 |
| y | -0.0768 | -0.2527 | -0.0085 | -0.1120 | 0.1656 | 0.0042 | -0.0337 | -0.1902 | -0.1644 |
| z | -0.0704 | -0.2511 | -0.1798 | -0.0061 | 0.0134 | -0.0243 | -0.2478 | 0.0483 | -0.0152 |
| Sn x | -0.0134 | -0.0587 | 0.1395 | -0.0390 | -0.0300 | -0.0645 | 0.1621 | -0.0482 | 0.0672 |
| y | -0.0332 | -0.0095 | 0.0005 | 0.1646 | 0.1113 | 0.0579 | 0.0256 | -0.0144 | 0.0982 |
| z | 0.1125 | 0.1736 | -0.1407 | 0.3309 | -0.1726 | -0.1561 | 0.0976 | 0.1325 | 0.0392 |
| Ag x | 0.0005 | 0.0791 | -0.1040 | 0.2470 | 0.1931 | -0.0861 | 0.1243 | -0.2041 | 0.0254 |
| y | -0.0334 | 0.0502 | -0.1406 | -0.0464 | -0.0491 | 0.0081 | -0.0182 | -0.0909 | 0.1238 |
| z | -0.2287 | 0.1555 | 0.1604 | 0.2157 | 0.1224 | -0.0006 | -0.0114 | 0.1911 | -0.0623 |
| Sn x | -0.0876 | 0.0553 | 0.0363 | 0.0749 | -0.0129 | 0.0144 | 0.1269 | -0.0498 | 0.0430 |
| y | -0.0818 | 0.0139 | 0.0296 | 0.1755 | -0.1258 | 0.0317 | -0.1592 | 0.0078 | -0.0627 |
| z | 0.1784 | -0.0611 | 0.1015 | -0.0839 | 0.0501 | -0.0440 | 0.2236 | 0.0546 | -0.0376 |

25: 62.8 26: 66.1 27: 69.9 28: 70.5 29: 72.5 30: 74.8 31: 75.9 32: 77.2 33: 84.6

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.1174 | 0.0347 | 0.0054 | 0.0629 | -0.0143 | -0.1077 | 0.0111 | 0.0019 | -0.0859 |
| y | -0.0386 | -0.0347 | -0.0072 | 0.0600 | 0.0834 | -0.0352 | -0.1098 | 0.0471 | 0.1489 |
| z | 0.1390 | 0.0697 | 0.1312 | -0.0608 | 0.0122 | 0.1252 | 0.0023 | -0.0468 | -0.0741 |
| Sn x | -0.2294 | 0.0658 | -0.1234 | -0.1127 | -0.0738 | -0.2491 | -0.1441 | -0.1308 | 0.0915 |
| y | 0.2310 | -0.1058 | 0.0632 | -0.0261 | 0.0472 | -0.3197 | -0.2261 | -0.2502 | 0.0839 |
| z | -0.2001 | -0.3099 | -0.1990 | -0.1831 | 0.1408 | 0.0604 | 0.2377 | 0.0007 | -0.0811 |
| Sn x | 0.2073 | 0.2451 | 0.0917 | 0.1473 | -0.1928 | -0.1155 | 0.2909 | 0.0618 | 0.2231 |
| y | -0.0708 | -0.0241 | -0.1839 | -0.0460 | 0.1519 | 0.0138 | -0.2144 | 0.1446 | 0.0548 |
| z | 0.0185 | -0.0507 | -0.0430 | 0.0677 | 0.0128 | -0.2080 | -0.0808 | -0.4068 | 0.0210 |
| Ag x | 0.2200 | -0.2013 | -0.0048 | 0.1186 | -0.2970 | 0.3310 | -0.1041 | -0.0129 | 0.0896 |
| y | -0.0780 | -0.0896 | -0.0684 | -0.1291 | -0.1036 | 0.0708 | -0.0314 | 0.0418 | -0.1341 |
| z | -0.0712 | 0.0519 | 0.2879 | -0.0221 | -0.1580 | 0.0605 | -0.0785 | 0.0386 | -0.1326 |
| Ag x | 0.1718 | 0.1174 | 0.0833 | -0.0161 | 0.1675 | -0.0058 | -0.2286 | -0.1329 | -0.1778 |
| y | 0.1004 | -0.0584 | -0.0616 | 0.1254 | -0.1018 | -0.1380 | -0.0303 | 0.0890 | 0.0675 |
| z | 0.1199 | -0.0742 | -0.0169 | 0.1830 | -0.1039 | 0.2498 | -0.1731 | -0.0790 | 0.1347 |
| Ag x | 0.3269 | 0.1906 | -0.0649 | -0.1215 | 0.0485 | -0.0214 | 0.0989 | -0.0333 | 0.0068 |
| y | -0.0534 | 0.0978 | 0.0794 | 0.3332 | 0.1598 | -0.0748 | 0.0238 | -0.0417 | -0.0774 |
| z | 0.0024 | -0.0062 | 0.0283 | -0.2551 | -0.0945 | 0.0749 | -0.1110 | 0.0075 | -0.0762 |
| Ag x | -0.0629 | -0.1815 | 0.1859 | -0.0325 | 0.1421 | 0.0463 | 0.1951 | -0.0503 | 0.0698 |
| y | 0.1817 | 0.0708 | 0.1510 | -0.2527 | 0.1999 | 0.1343 | 0.1607 | -0.0386 | 0.0443 |
| z | -0.0110 | 0.0466 | -0.0793 | -0.0743 | -0.0795 | -0.0067 | 0.1396 | 0.0230 | -0.1166 |
| Ag x | -0.1263 | -0.0804 | -0.1479 | -0.0712 | -0.1467 | -0.0033 | -0.1762 | -0.1101 | -0.0093 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| y | -0.0415 | -0.0827 | 0.1934 | -0.1570 | 0.0026 | 0.0268 | 0.0129 | 0.0104 | -0.0172 |
| z | 0.0044 | -0.1776 | -0.0789 | -0.0552 | -0.1065 | -0.0604 | -0.0571 | 0.1522 | 0.2086 |
| Ag x | -0.1958 | 0.0092 | 0.1772 | -0.2159 | -0.0775 | -0.0460 | -0.0015 | 0.0502 | -0.0668 |
| y | -0.1112 | 0.1425 | 0.0512 | -0.0780 | 0.0295 | -0.0535 | 0.0744 | 0.0394 | -0.0128 |
| z | -0.0466 | 0.1263 | -0.0245 | -0.1292 | 0.1296 | -0.0524 | 0.2074 | 0.0352 | 0.2382 |
| Sn x | 0.2937 | -0.0450 | 0.0024 | 0.0131 | -0.0047 | -0.0684 | -0.0456 | 0.4256 | -0.0782 |
| y | -0.0247 | 0.1551 | -0.0639 | 0.1392 | 0.0515 | 0.1295 | 0.0544 | 0.0105 | 0.0551 |
| z | 0.1761 | -0.1677 | 0.0543 | 0.2048 | 0.0177 | -0.1671 | 0.0799 | 0.3242 | -0.2633 |
| Sn x | -0.0569 | -0.0181 | -0.2401 | 0.0369 | 0.3045 | 0.0505 | -0.2348 | -0.0778 | -0.2256 |
| y | -0.1153 | -0.1486 | 0.0838 | 0.0449 | -0.2457 | -0.0622 | 0.0979 | 0.0568 | 0.2149 |
| z | 0.0721 | 0.1376 | -0.1356 | 0.0120 | 0.0413 | -0.1020 | 0.1432 | -0.0347 | -0.0043 |
| Sn x | -0.1639 | -0.0420 | 0.0899 | 0.2097 | 0.0738 | -0.0240 | -0.0193 | -0.0102 | 0.0195 |
| y | -0.0446 | 0.1117 | -0.0746 | -0.0175 | 0.0350 | -0.1185 | 0.1067 | 0.0274 | 0.1526 |
| z | 0.0229 | 0.0880 | -0.1287 | 0.0810 | -0.1774 | -0.3139 | -0.0596 | -0.0188 | -0.2100 |
| Sn x | 0.0079 | -0.3001 | 0.0852 | -0.0704 | -0.1175 | -0.0064 | 0.0443 | -0.0429 | 0.0801 |
| y | 0.0214 | -0.0268 | -0.0127 | -0.0170 | 0.1633 | -0.1155 | 0.0179 | 0.2324 | -0.1990 |
| z | 0.1034 | 0.0074 | 0.2376 | -0.0180 | -0.0490 | -0.0257 | 0.0644 | -0.1814 | -0.0103 |
| Ag x | -0.0425 | 0.0166 | -0.2296 | -0.0696 | -0.2857 | -0.0313 | 0.0463 | 0.1102 | -0.0932 |
| y | 0.0756 | -0.3520 | -0.0719 | 0.1226 | -0.0301 | 0.0985 | 0.2785 | -0.1659 | -0.2362 |
| z | 0.0402 | -0.0145 | 0.0127 | -0.0112 | 0.1220 | 0.1490 | -0.2279 | 0.0573 | 0.3642 |
| Ag x | 0.0744 | 0.1647 | -0.0731 | -0.1266 | 0.0657 | -0.1262 | 0.0463 | 0.0827 | 0.1156 |
| y | 0.3106 | 0.0435 | -0.1470 | -0.2301 | 0.0262 | 0.2601 | -0.0133 | -0.1667 | -0.1261 |
| z | -0.0794 | -0.0079 | -0.1149 | 0.3934 | 0.1046 | 0.0714 | 0.0730 | -0.0869 | 0.1034 |
| Sn x | -0.2201 | -0.0854 | 0.2080 | 0.0216 | 0.2345 | 0.1375 | 0.1011 | 0.1229 | 0.0443 |
| y | -0.1569 | 0.3153 | -0.1749 | 0.0743 | -0.2311 | 0.3076 | -0.0669 | 0.1039 | 0.0426 |
| z | -0.0410 | -0.0819 | -0.2639 | -0.1707 | 0.1371 | -0.0110 | -0.0410 | 0.1320 | 0.1755 |
| Ag x | 0.0353 | -0.0509 | 0.1491 | 0.1181 | 0.2007 | 0.0601 | -0.1546 | -0.0057 | 0.1251 |
| y | -0.0292 | -0.0564 | 0.0037 | 0.1728 | -0.0166 | -0.0079 | -0.0241 | 0.0064 | -0.0534 |
| z | -0.0921 | 0.1521 | 0.1295 | -0.0074 | 0.0677 | 0.0244 | 0.0944 | -0.0878 | -0.0030 |
| Sn x | -0.1033 | 0.1597 | -0.1908 | 0.0889 | -0.0358 | 0.1892 | 0.2619 | -0.2533 | -0.1257 |
| y | -0.1401 | 0.0290 | 0.2464 | -0.1232 | -0.2136 | -0.1015 | -0.0898 | -0.1572 | -0.0339 |
| z | -0.1636 | 0.2154 | 0.2100 | 0.0462 | -0.0226 | 0.1555 | -0.2190 | 0.1744 | -0.2405 |

34: 84.8 35: 86.5 36: 88.2 37: 91.3 38: 95.9 39: 96.6 40: 102.2 41: 105.6 42: 106.5

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.0238 | 0.0502 | -0.0107 | 0.0768 | -0.0941 | -0.0829 | -0.0435 | -0.0064 | -0.0624 |
| y | -0.1050 | -0.0726 | 0.1197 | -0.0358 | -0.0729 | 0.0670 | -0.0738 | 0.2662 | -0.1248 |
| z | 0.1683 | 0.0714 | -0.1922 | -0.1392 | -0.0009 | 0.0097 | 0.0333 | -0.0309 | 0.1731 |
| Sn x | -0.0503 | 0.0663 | -0.1510 | 0.0027 | 0.0997 | 0.1354 | -0.0140 | -0.0102 | 0.0223 |
| y | 0.0796 | -0.0160 | 0.0443 | 0.0396 | 0.0624 | -0.2316 | 0.2631 | -0.0987 | 0.0480 |
| z | -0.0377 | -0.1793 | -0.0877 | 0.0402 | -0.2099 | 0.1990 | 0.2673 | 0.1421 | -0.0047 |
| Sn x | -0.0275 | -0.0648 | -0.3011 | 0.1663 | 0.1635 | -0.0010 | -0.0815 | 0.2149 | -0.0258 |
| y | 0.0559 | 0.1433 | -0.0462 | 0.0793 | 0.0747 | -0.1567 | -0.3756 | -0.2133 | 0.0526 |
| z | 0.0587 | 0.2245 | 0.1398 | -0.2363 | 0.0705 | 0.1715 | -0.2500 | -0.0220 | -0.0886 |
| Ag x | 0.0423 | 0.2212 | -0.0514 | 0.1619 | 0.0093 | -0.0363 | -0.0213 | 0.2074 | 0.2408 |
| y | -0.0787 | -0.0222 | -0.0469 | 0.1832 | -0.2791 | 0.1994 | 0.0105 | 0.0703 | 0.0945 |
| z | 0.0389 | -0.1175 | -0.0812 | 0.0673 | 0.1928 | 0.0968 | -0.0309 | -0.1121 | -0.0200 |
| Ag x | 0.3277 | -0.3076 | 0.0524 | 0.2456 | -0.1020 | 0.0399 | 0.2664 | -0.0810 | -0.0231 |
| y | -0.0673 | 0.0399 | 0.0724 | -0.0281 | -0.1521 | -0.0462 | 0.3447 | 0.1084 | -0.1570 |
| z | 0.0059 | 0.0703 | 0.0711 | 0.0128 | -0.2388 | 0.0696 | -0.1651 | -0.1541 | -0.2771 |
| Ag x | -0.1516 | -0.1692 | 0.1059 | 0.0204 | -0.0104 | 0.0395 | -0.0943 | 0.0835 | -0.1214 |
| y | -0.0611 | 0.0675 | -0.1221 | 0.0045 | -0.0121 | 0.0549 | 0.1219 | -0.0036 | -0.0395 |
| z | 0.0897 | 0.2366 | -0.1125 | -0.0522 | -0.1218 | -0.0554 | 0.0076 | 0.1604 | -0.2053 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Ag x | -0.0709 | -0.0017 | -0.0188 | -0.0261 | 0.0315 | -0.1081 | 0.0482 | 0.0043 | -0.1330 |
| y | -0.1832 | -0.2036 | 0.1458 | -0.0049 | -0.1495 | -0.0162 | -0.3252 | 0.0110 | 0.1318 |
| z | -0.0127 | -0.0539 | 0.0035 | -0.0744 | 0.1757 | -0.0762 | -0.1011 | 0.0002 | -0.0719 |
| Ag x | 0.1584 | -0.2700 | -0.0799 | -0.0899 | -0.1332 | -0.1290 | -0.1268 | 0.1792 | -0.0690 |
| y | 0.0366 | 0.2507 | 0.0766 | 0.0940 | 0.0900 | 0.0302 | 0.1417 | 0.1093 | -0.3073 |
| z | -0.1052 | -0.1319 | 0.3399 | 0.2038 | 0.1537 | 0.1288 | -0.0088 | -0.0678 | 0.0203 |
| Ag x | 0.1714 | -0.0499 | 0.0100 | 0.0330 | 0.0127 | 0.0386 | -0.0214 | -0.0047 | 0.0159 |
| y | 0.0570 | -0.0589 | 0.0059 | -0.0056 | 0.0316 | 0.0581 | 0.0182 | -0.1514 | -0.0876 |
| z | 0.3860 | 0.0925 | 0.1192 | -0.0562 | 0.0579 | -0.0994 | -0.0067 | 0.0181 | 0.0147 |
| Sn x | 0.0019 | 0.1007 | 0.2317 | 0.0271 | 0.0007 | 0.3542 | -0.0253 | -0.2294 | -0.0651 |
| y | 0.1606 | -0.0143 | -0.2865 | 0.1098 | -0.1746 | 0.1361 | -0.1108 | -0.2005 | -0.2075 |
| z | 0.2000 | -0.1029 | -0.1901 | -0.3159 | -0.1588 | -0.0766 | -0.1402 | 0.1455 | -0.0002 |
| Sn x | -0.1613 | -0.0679 | -0.0162 | 0.0125 | 0.1819 | -0.0102 | -0.1512 | 0.1109 | 0.0210 |
| y | 0.1479 | -0.2121 | 0.0680 | 0.0166 | -0.0782 | 0.0048 | -0.1049 | -0.1673 | 0.3349 |
| z | -0.2919 | -0.0523 | -0.1795 | -0.1315 | -0.0531 | 0.0234 | 0.1769 | -0.2406 | 0.2351 |
| Sn x | 0.0138 | -0.0358 | -0.0043 | -0.0374 | 0.0804 | 0.0637 | 0.0269 | -0.0311 | 0.1272 |
| y | 0.2432 | 0.1351 | 0.1107 | -0.0083 | -0.0456 | -0.1520 | -0.0355 | 0.1587 | 0.1144 |
| z | -0.1010 | 0.1552 | 0.0542 | 0.2181 | -0.3062 | -0.0826 | -0.0800 | 0.0587 | 0.1046 |
| Sn x | -0.2040 | 0.0725 | 0.0738 | -0.2247 | -0.1250 | -0.3098 | 0.0792 | -0.1923 | 0.1263 |
| y | 0.0051 | 0.1467 | 0.1395 | -0.0499 | 0.2391 | 0.0866 | 0.0328 | 0.3180 | 0.2051 |
| z | -0.0977 | -0.1712 | 0.1262 | 0.1108 | 0.1101 | -0.1784 | -0.0503 | 0.1674 | -0.1570 |
| Ag x | 0.0109 | 0.0863 | -0.0677 | 0.0379 | 0.2952 | -0.0144 | 0.1069 | -0.1172 | -0.0975 |
| y | 0.0380 | -0.0717 | 0.0100 | -0.0484 | 0.2707 | 0.0019 | -0.0379 | -0.2054 | -0.2324 |
| z | 0.0426 | 0.0012 | -0.1145 | -0.2642 | 0.1550 | 0.2949 | 0.2138 | 0.0547 | 0.0809 |
| Ag x | -0.1951 | 0.0978 | -0.0022 | -0.2677 | -0.1643 | -0.0466 | 0.0485 | -0.1512 | -0.1612 |
| y | -0.0391 | 0.1658 | -0.1825 | 0.0254 | 0.0949 | -0.0647 | 0.0849 | -0.0010 | 0.2120 |
| z | -0.1519 | -0.0224 | 0.0466 | 0.1897 | 0.0887 | -0.0294 | -0.0009 | 0.1623 | 0.0533 |
| Sn x | -0.0989 | 0.2737 | -0.0955 | 0.1053 | -0.0958 | -0.1411 | -0.0232 | 0.0008 | -0.0229 |
| y | -0.1043 | -0.1489 | 0.1461 | -0.2237 | 0.0087 | -0.1816 | 0.1678 | 0.0721 | -0.1546 |
| z | 0.0127 | -0.1565 | -0.1826 | 0.2150 | 0.1028 | -0.1799 | -0.0198 | -0.0518 | -0.0535 |
| Ag x | 0.0074 | -0.0905 | -0.0234 | -0.0991 | -0.0714 | 0.0259 | -0.0032 | 0.0266 | 0.0509 |
| y | 0.0368 | -0.0684 | -0.0941 | -0.0164 | 0.0577 | -0.0887 | 0.0178 | -0.1809 | 0.0480 |
| z | -0.0900 | 0.2040 | 0.0746 | 0.3106 | -0.0771 | 0.0409 | 0.0963 | -0.1640 | 0.0700 |
| Sn x | 0.2158 | 0.0663 | 0.3449 | -0.1439 | -0.0850 | 0.1732 | 0.0390 | 0.0026 | 0.1632 |
| y | -0.2341 | -0.0556 | -0.1669 | -0.1218 | 0.0320 | 0.3046 | -0.1221 | 0.0967 | 0.0536 |
| z | -0.1051 | -0.0549 | 0.1815 | -0.0825 | 0.0773 | -0.2394 | 0.0586 | -0.0707 | 0.1108 |

43: 110.3 44: 114.3 45: 116.4 46: 118.0 47: 120.5 48: 123.7 49: 125.6 50: 132.1 51: 133.5

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.1032 | 0.1397 | -0.2415 | -0.0592 | 0.1876 | -0.0568 | -0.3212 | 0.0200 | -0.0741 |
| y | -0.4340 | 0.0809 | 0.2081 | -0.0545 | 0.0150 | -0.0379 | -0.1152 | -0.0019 | -0.0606 |
| z | -0.0155 | -0.0284 | 0.3926 | 0.1444 | -0.0299 | 0.0002 | -0.0057 | 0.0206 | -0.0210 |
| Sn x | -0.0017 | 0.0617 | -0.0511 | 0.0433 | -0.1787 | -0.1322 | -0.0484 | 0.1320 | -0.0440 |
| y | -0.1041 | 0.0206 | -0.0556 | 0.0006 | -0.2043 | -0.1979 | -0.1002 | 0.3126 | -0.0244 |
| z | 0.0959 | 0.0820 | 0.0119 | 0.0104 | -0.1467 | -0.0108 | -0.0404 | -0.0220 | 0.0139 |
| Sn x | 0.0509 | -0.1503 | 0.0195 | 0.0042 | 0.1039 | 0.1262 | 0.0044 | -0.0383 | 0.0583 |
| y | -0.1659 | -0.0558 | -0.0339 | 0.0312 | 0.1860 | 0.2782 | 0.0844 | -0.0693 | -0.0158 |
| z | 0.1266 | 0.0009 | 0.0665 | -0.0572 | 0.1635 | -0.2317 | 0.1320 | -0.2779 | -0.0352 |
| Ag x | 0.0030 | 0.0930 | -0.0631 | 0.0491 | -0.0018 | -0.1309 | 0.0265 | 0.1014 | -0.0711 |
| y | -0.0188 | -0.1031 | 0.0250 | 0.0967 | 0.2021 | -0.0604 | 0.0361 | 0.0150 | 0.0411 |
| z | -0.1149 | -0.0323 | 0.0152 | -0.0476 | 0.1965 | -0.0058 | 0.0345 | 0.0307 | 0.0551 |
| Ag x | -0.0769 | 0.0247 | 0.0034 | -0.0290 | 0.0677 | 0.0211 | 0.0071 | -0.4936 | 0.0975 |
| y | 0.1409 | -0.0979 | 0.1716 | -0.0932 | 0.1641 | 0.2991 | -0.0596 | 0.1382 | 0.2344 |

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|---|---|---|---|---|---|---|---|---|---|
| z | 0.0965 | -0.0298 | 0.0994 | 0.0208 | 0.0576 | 0.1527 | -0.1008 | 0.0123 | 0.1597 |
| Ag x | -0.1494 | 0.1567 | -0.1467 | -0.1252 | 0.1191 | -0.0416 | 0.0321 | 0.0596 | 0.0532 |
| y | -0.0980 | 0.1634 | 0.0472 | -0.0306 | 0.1499 | 0.0070 | 0.0634 | 0.0603 | -0.0711 |
| z | -0.1528 | -0.0525 | -0.1113 | -0.1600 | 0.0057 | 0.0072 | -0.2645 | -0.0820 | -0.1199 |
| Ag x | 0.0406 | 0.0541 | 0.0385 | 0.3900 | 0.1639 | 0.0632 | -0.0668 | -0.0467 | -0.4435 |
| y | 0.0500 | -0.0168 | -0.0502 | -0.1776 | -0.1083 | -0.0688 | 0.1154 | 0.0870 | 0.0179 |
| z | -0.0958 | 0.1057 | -0.0555 | 0.3745 | 0.0006 | -0.1626 | -0.1858 | -0.0229 | 0.5177 |
| Ag x | -0.0046 | -0.0721 | -0.1476 | -0.1338 | -0.0859 | 0.0410 | 0.3571 | 0.0869 | 0.0683 |
| y | -0.0579 | 0.0306 | -0.1316 | 0.1981 | -0.0092 | 0.0348 | 0.2707 | 0.0225 | 0.0271 |
| z | 0.0843 | 0.0108 | -0.0095 | 0.0838 | -0.0511 | 0.0022 | 0.1982 | 0.0333 | 0.0795 |
| Ag x | 0.0282 | 0.0922 | 0.0341 | -0.0189 | 0.1049 | -0.0012 | 0.0299 | 0.0502 | 0.0206 |
| y | -0.1296 | -0.4421 | -0.0259 | 0.0244 | 0.1070 | -0.2502 | -0.0069 | 0.1915 | -0.0787 |
| z | 0.0517 | 0.0563 | 0.0093 | -0.0309 | 0.0155 | -0.0638 | 0.0076 | 0.0899 | -0.0256 |
| Sn x | 0.0615 | 0.1737 | 0.0298 | 0.0924 | -0.1402 | -0.1473 | -0.0429 | 0.0292 | -0.1592 |
| y | -0.0485 | 0.1591 | 0.0051 | 0.0596 | -0.1987 | -0.0408 | 0.0116 | 0.1595 | 0.0077 |
| z | 0.0264 | -0.0450 | -0.0999 | -0.1160 | -0.0889 | -0.0376 | 0.1465 | 0.0683 | -0.1693 |
| Sn x | 0.2994 | 0.0120 | 0.2640 | -0.0750 | 0.0637 | 0.0335 | -0.2259 | 0.2101 | -0.0231 |
| y | 0.0177 | -0.0976 | 0.1335 | -0.1135 | -0.0331 | -0.0660 | -0.4144 | -0.1664 | -0.0539 |
| z | -0.1178 | 0.2676 | 0.0144 | -0.0492 | 0.2572 | -0.0327 | 0.1230 | 0.0309 | 0.0514 |
| Sn x | -0.0901 | -0.1690 | 0.3287 | 0.1233 | -0.2105 | 0.0465 | 0.3183 | -0.0180 | 0.0648 |
| y | 0.1602 | 0.4393 | 0.0960 | -0.0050 | -0.1171 | 0.1893 | 0.0605 | -0.1210 | 0.0683 |
| z | -0.0188 | -0.1264 | 0.0737 | 0.1616 | -0.0178 | -0.0822 | 0.0586 | 0.0342 | -0.0277 |
| Sn x | -0.1675 | 0.0405 | -0.0381 | -0.0472 | 0.1874 | 0.0423 | 0.1148 | -0.0853 | 0.0268 |
| y | 0.0423 | -0.1917 | -0.0798 | -0.0417 | 0.1441 | 0.0155 | -0.0286 | -0.1691 | 0.0702 |
| z | 0.1837 | -0.0862 | 0.1619 | -0.0060 | -0.0486 | 0.0619 | -0.0861 | 0.1353 | -0.0350 |
| Ag x | -0.0824 | 0.0192 | 0.1175 | -0.3057 | -0.1003 | 0.0529 | 0.0229 | -0.0416 | -0.0369 |
| y | -0.0589 | 0.0270 | 0.0252 | -0.2134 | -0.0925 | 0.0732 | -0.0338 | -0.0437 | 0.0012 |
| z | 0.0161 | -0.0787 | -0.1884 | -0.1594 | 0.0803 | 0.0476 | -0.0527 | 0.1034 | 0.0558 |
| Ag x | 0.0638 | -0.3120 | -0.0249 | 0.0948 | -0.3145 | 0.1790 | -0.1086 | -0.2469 | 0.0292 |
| y | 0.0365 | -0.1001 | 0.0116 | 0.0989 | -0.1585 | -0.0195 | 0.0153 | -0.1028 | -0.0325 |
| z | -0.2471 | -0.0695 | -0.2749 | 0.0136 | -0.2502 | -0.0624 | -0.0678 | -0.2410 | -0.0905 |
| Sn x | 0.0156 | -0.0119 | 0.0836 | -0.2250 | -0.0793 | -0.3067 | -0.0128 | -0.0284 | 0.3974 |
| y | 0.2029 | 0.0464 | 0.1160 | 0.0101 | 0.0776 | -0.3757 | 0.1185 | -0.1673 | -0.2044 |
| z | -0.0271 | -0.0352 | 0.0297 | 0.1243 | 0.1118 | 0.0976 | 0.0318 | -0.0210 | -0.1683 |
| Ag x | 0.0661 | -0.0159 | -0.0918 | 0.1165 | 0.0481 | -0.0281 | -0.0146 | 0.0170 | 0.0278 |
| y | 0.4090 | -0.0689 | -0.3947 | 0.1585 | 0.0410 | -0.0200 | 0.0297 | -0.0018 | 0.1251 |
| z | 0.2094 | -0.0782 | -0.0648 | -0.3397 | -0.0289 | 0.1032 | 0.1412 | 0.0073 | -0.1974 |
| Sn x | -0.1649 | -0.1343 | -0.1273 | 0.1072 | 0.0651 | 0.2464 | -0.0583 | 0.2685 | -0.0039 |
| y | 0.0690 | 0.1782 | -0.0825 | 0.0542 | -0.1511 | 0.2399 | -0.0270 | -0.1263 | -0.0393 |
| z | -0.1080 | 0.1311 | -0.0977 | 0.0211 | -0.2253 | 0.2179 | -0.0832 | 0.0975 | -0.0230 |

52: 139.9 53: 141.3 54: 146.1

| | | | |
|---|---|---|---|
| Sn x | -0.0583 | 0.4911 | -0.0791 |
| y | -0.0109 | 0.1434 | -0.0183 |
| z | -0.0133 | 0.3689 | -0.0355 |
| Sn x | 0.2023 | 0.0069 | -0.0069 |
| y | 0.2425 | -0.0188 | -0.1254 |
| z | 0.0129 | 0.0047 | 0.1055 |
| Sn x | 0.1201 | 0.0354 | 0.0336 |
| y | -0.1798 | -0.0033 | 0.0089 |
| z | -0.1704 | -0.0134 | -0.0404 |
| Ag x | -0.1032 | 0.0014 | 0.2005 |

| | | | |
|---|---|---|---|
| y | 0.0369 | -0.0498 | -0.3189 |
| z | 0.1263 | -0.0761 | -0.5188 |
| Ag x | -0.0685 | 0.0385 | 0.1551 |
| y | -0.2829 | -0.0325 | 0.0046 |
| z | 0.5661 | 0.0638 | 0.2040 |
| Ag x | 0.0276 | -0.2758 | 0.0720 |
| y | 0.0146 | -0.0062 | 0.0402 |
| z | 0.0143 | -0.4592 | 0.0344 |
| Ag x | 0.1028 | -0.0772 | 0.0006 |
| y | 0.0614 | 0.0731 | -0.0200 |
| z | -0.0846 | -0.0492 | 0.0339 |
| Ag x | 0.0167 | 0.1466 | -0.0198 |
| y | -0.0022 | 0.1034 | -0.0080 |
| z | -0.0127 | 0.1595 | -0.0097 |
| Ag x | 0.0250 | -0.0258 | -0.0152 |
| y | -0.1098 | 0.0544 | 0.3658 |
| z | -0.0417 | 0.0025 | 0.2137 |
| Sn x | -0.1311 | -0.0531 | -0.0505 |
| y | -0.1743 | -0.0374 | -0.0591 |
| z | 0.0011 | 0.0117 | -0.0536 |
| Sn x | -0.0493 | -0.0961 | -0.0017 |
| y | -0.0081 | -0.1329 | 0.0053 |
| z | 0.0919 | -0.0119 | 0.0962 |
| Sn x | 0.0491 | -0.3310 | 0.0555 |
| y | 0.0901 | -0.1025 | -0.1840 |
| z | -0.0335 | -0.0225 | 0.1038 |
| Sn x | -0.1082 | -0.0061 | 0.0116 |
| y | 0.3544 | 0.0613 | 0.0969 |
| z | -0.2895 | -0.0335 | -0.0907 |
| Ag x | -0.0170 | 0.0632 | 0.0247 |
| y | 0.0830 | 0.0571 | 0.0487 |
| z | -0.1318 | 0.0172 | -0.0742 |
| Ag x | 0.0389 | 0.1059 | -0.2111 |
| y | -0.0661 | 0.0588 | -0.0811 |
| z | -0.0962 | 0.0272 | -0.1473 |
| Sn x | -0.0283 | 0.0186 | -0.0233 |
| y | 0.0580 | -0.0134 | -0.0508 |
| z | 0.0408 | -0.0138 | -0.0036 |
| Ag x | -0.0150 | -0.0242 | -0.0006 |
| y | -0.0109 | -0.1967 | 0.0162 |
| z | 0.0313 | -0.0195 | -0.0032 |
| Sn x | -0.0034 | -0.0207 | -0.1359 |
| y | -0.1086 | 0.0449 | 0.2811 |
| z | 0.0065 | 0.0281 | 0.1731 |