$coordinates

| | | | |
|---|---|---|---|
| Sn | 1.01690051086380 | 4.62490031137221 | -4.02833392386141 |
| Sn | 0.49108482507614 | -6.57904040073224 | -0.78459020820705 |
| Sn | 4.56042068658184 | -1.27559415489477 | -2.05196931734536 |
| Ag | -4.37954042370110 | 3.50503571609966 | -2.64701221332338 |
| Ag | 1.33068834717098 | 2.04153539674691 | 0.89968661401773 |
| Ag | 1.30816323316998 | -4.10115444449899 | -5.44906449512584 |
| Ag | -2.41835319602165 | -2.27502047221569 | 1.37936561912125 |
| Ag | -4.01572130021892 | -4.29418463724969 | -3.43598083003464 |
| Ag | -7.35665491738519 | -0.16248967310971 | -5.46518820345239 |
| Sn | -4.72883356639061 | 2.98575316690490 | 2.85587937113788 |
| Sn | -7.54863560915840 | -1.17725955178265 | -0.17195135229357 |
| Sn | 3.16448789899401 | -3.30538064622189 | 3.08958769696134 |
| Ag | -2.08173280050101 | 0.19150735884260 | -6.41694064804198 |
| Sn | -1.11266341781777 | 7.06944850354467 | 0.53750326959469 |
| Sn | 3.25228468247560 | 0.96093990372573 | -7.53191999514579 |
| Ag | -0.35831875434194 | 0.30633331271944 | 5.67096983156781 |

$end

vibrational frequencies, intensities

| mode | au_amu | cm-1 | km/mol |
|---|---|---|---|
| 7 | 0.004175 | 21.5 | 0.09 |
| 8 | 0.005242 | 26.9 | 0.08 |
| 9 | 0.005813 | 29.9 | 0.05 |
| 10 | 0.006021 | 31.0 | 0.02 |
| 11 | 0.006491 | 33.4 | 0.12 |
| 12 | 0.007334 | 37.7 | 0.27 |
| 13 | 0.007829 | 40.2 | 0.02 |
| 14 | 0.008288 | 42.6 | 0.12 |
| 15 | 0.008935 | 45.9 | 0.30 |
| 16 | 0.008984 | 46.2 | 0.00 |
| 17 | 0.009857 | 50.7 | 0.05 |
| 18 | 0.010414 | 53.5 | 0.25 |
| 19 | 0.010651 | 54.8 | 0.08 |
| 20 | 0.011263 | 57.9 | 0.07 |
| 21 | 0.012030 | 61.8 | 0.13 |
| 22 | 0.012106 | 62.2 | 0.02 |
| 23 | 0.012594 | 64.7 | 0.12 |
| 24 | 0.012947 | 66.6 | 0.22 |
| 25 | 0.013541 | 69.6 | 0.11 |
| 26 | 0.014237 | 73.2 | 0.11 |
| 27 | 0.015137 | 77.8 | 0.22 |
| 28 | 0.015704 | 80.7 | 0.57 |
| 29 | 0.016221 | 83.4 | 0.25 |
| 30 | 0.017356 | 89.2 | 0.24 |
| 31 | 0.018081 | 92.9 | 0.10 |
| 32 | 0.018182 | 93.5 | 0.00 |
| 33 | 0.018419 | 94.7 | 0.09 |
| 34 | 0.019419 | 99.8 | 0.02 |
| 35 | 0.020416 | 104.9 | 0.51 |
| 36 | 0.020754 | 106.7 | 0.27 |

| | | | |
|---|---|---|---|
| 37 | 0.021811 | 112.1 | 0.09 |
| 38 | 0.022978 | 118.1 | 0.53 |
| 39 | 0.023427 | 120.4 | 0.26 |
| 40 | 0.024553 | 126.2 | 0.63 |
| 41 | 0.024980 | 128.4 | 0.19 |
| 42 | 0.025175 | 129.4 | 0.05 |
| 43 | 0.026411 | 135.8 | 0.32 |
| 44 | 0.027107 | 139.3 | 0.26 |
| 45 | 0.027963 | 143.7 | 0.56 |
| 46 | 0.028742 | 147.7 | 0.22 |
| 47 | 0.029408 | 151.2 | 0.09 |
| 48 | 0.033754 | 173.5 | 0.87 |

Frequencies (cm-1) and normal modes

| 7: 21.5 | 8: 26.9 | 9: 29.9 | 10: 31.0 | 11: 33.4 | 12: 37.7 | 13: 40.2 | 14: 42.6 | 15: 45.9 |
|---|---|---|---|---|---|---|---|---|
| Sn x 0.0101 | 0.0458 | -0.1211 | -0.1033 | 0.0459 | 0.1681 | 0.0406 | 0.1690 | 0.2373 |
| y 0.0834 | -0.3065 | 0.1113 | -0.0836 | 0.0184 | 0.0030 | -0.0535 | -0.1234 | 0.2154 |
| z -0.1441 | 0.0767 | 0.0039 | 0.0016 | -0.0450 | 0.1305 | 0.0509 | -0.1116 | 0.1774 |
| Sn x -0.0759 | 0.0569 | -0.2199 | -0.2059 | 0.1532 | 0.0426 | 0.1903 | -0.0990 | -0.3143 |
| y -0.0355 | 0.0638 | -0.1691 | 0.1235 | -0.0893 | 0.0279 | 0.0162 | 0.0117 | -0.0842 |
| z -0.0104 | -0.0304 | 0.0186 | 0.1251 | -0.1656 | 0.1096 | 0.1796 | 0.0686 | -0.0182 |
| Sn x 0.0190 | 0.0624 | -0.2295 | 0.0917 | -0.3051 | -0.3702 | -0.0318 | -0.0196 | 0.0239 |
| y 0.1967 | 0.3148 | 0.0063 | -0.0480 | -0.1208 | 0.1528 | -0.0936 | 0.1707 | 0.0428 |
| z 0.0719 | 0.1387 | 0.0452 | 0.0088 | 0.1354 | -0.3032 | 0.0094 | -0.0149 | 0.0084 |
| Ag x -0.0438 | -0.0155 | -0.1286 | 0.0055 | 0.0911 | 0.2258 | -0.2413 | 0.1292 | 0.3343 |
| y 0.0950 | -0.0333 | 0.0356 | -0.3552 | -0.0609 | -0.1128 | 0.4705 | 0.0137 | 0.0376 |
| z -0.0580 | -0.0998 | -0.0372 | 0.0796 | -0.0126 | -0.0278 | -0.2786 | 0.1745 | -0.2874 |
| Ag x -0.5953 | 0.0356 | 0.0569 | 0.1294 | -0.0999 | -0.0732 | 0.0421 | -0.0580 | 0.0320 |
| y -0.1954 | 0.1083 | 0.3255 | -0.0265 | 0.1493 | 0.0261 | -0.0520 | 0.1068 | 0.0520 |
| z -0.2191 | 0.3767 | 0.0949 | -0.0196 | 0.0690 | 0.2556 | 0.0425 | 0.0233 | 0.0075 |
| Ag x 0.1303 | 0.1372 | -0.0347 | -0.1263 | -0.2579 | -0.2063 | -0.3061 | 0.1537 | 0.0675 |
| y 0.0696 | 0.2126 | -0.1858 | 0.1523 | 0.0606 | -0.2585 | 0.0692 | -0.1282 | 0.0557 |
| z 0.0901 | 0.1154 | 0.0556 | 0.1078 | -0.1981 | -0.1293 | 0.0999 | 0.0658 | 0.1169 |
| Ag x -0.1876 | 0.0389 | 0.1402 | -0.0882 | 0.1688 | -0.0670 | 0.0671 | 0.0072 | 0.0243 |
| y -0.2627 | 0.0880 | 0.2200 | 0.1693 | -0.1672 | -0.0836 | -0.0606 | 0.0408 | 0.0323 |
| z 0.3024 | -0.1169 | -0.2017 | 0.1657 | 0.0427 | 0.2010 | 0.0822 | -0.0020 | 0.1162 |
| Ag x 0.0642 | 0.0125 | -0.0858 | -0.0027 | 0.0835 | -0.0107 | -0.0033 | 0.0231 | -0.0211 |
| y 0.0752 | 0.0294 | -0.1046 | 0.2143 | 0.1078 | -0.0240 | 0.0160 | 0.1933 | -0.0703 |
| z 0.0629 | -0.0481 | 0.0033 | 0.0353 | -0.0305 | 0.1742 | 0.0409 | -0.1241 | 0.0296 |
| Ag x 0.0868 | -0.1573 | 0.0748 | 0.0121 | 0.0058 | 0.1664 | -0.0327 | -0.0082 | -0.0103 |
| y -0.0487 | -0.0408 | -0.0617 | -0.1019 | -0.0186 | -0.0179 | 0.1285 | 0.5458 | -0.0848 |
| z -0.0022 | -0.0164 | -0.1363 | -0.2415 | 0.2081 | -0.1415 | -0.0920 | 0.1397 | 0.2232 |
| Sn x 0.1222 | 0.1630 | 0.1175 | -0.0785 | 0.0806 | -0.0714 | -0.0375 | -0.1835 | -0.0898 |
| y 0.0543 | 0.0738 | -0.0109 | -0.0677 | 0.0047 | 0.0258 | -0.2079 | -0.2362 | -0.0270 |
| z 0.0069 | -0.0641 | 0.0406 | 0.1414 | 0.0145 | -0.0115 | -0.2817 | 0.1353 | -0.3430 |
| Sn x 0.0024 | 0.0255 | 0.0709 | -0.0862 | 0.1604 | 0.0099 | 0.0268 | -0.0660 | -0.0076 |
| y 0.1414 | 0.1033 | 0.0926 | 0.0310 | -0.0904 | 0.0994 | -0.1572 | -0.2799 | -0.2891 |
| z 0.0367 | 0.0051 | -0.0711 | -0.1154 | 0.2325 | -0.1093 | -0.1821 | 0.0058 | 0.1115 |
| Sn x 0.0421 | -0.0284 | 0.0703 | 0.0869 | -0.0670 | 0.2229 | 0.2262 | 0.0345 | -0.1133 |
| y -0.1133 | -0.1060 | -0.1773 | -0.0389 | -0.0727 | 0.2377 | 0.0464 | 0.0473 | -0.1673 |
| z -0.0586 | 0.0397 | -0.1063 | 0.0216 | 0.1055 | -0.1782 | 0.1301 | -0.0637 | -0.0687 |
| Ag x 0.0739 | -0.1899 | 0.1338 | -0.0303 | -0.0489 | 0.1168 | -0.0944 | 0.0727 | -0.0549 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| y | 0.0420 | -0.0706 | -0.0859 | 0.1315 | 0.2154 | -0.0712 | 0.2152 | -0.0276 | -0.1225 |
| z | 0.0205 | -0.2028 | 0.2004 | -0.4746 | -0.3806 | -0.0722 | 0.0174 | 0.0679 | -0.1661 |
| Sn x | 0.0083 | 0.0766 | -0.2712 | -0.0941 | -0.1438 | 0.0205 | -0.0137 | -0.2672 | -0.0620 |
| y | 0.0869 | 0.0691 | 0.2066 | -0.1768 | 0.1519 | -0.0077 | -0.0969 | -0.0905 | 0.1031 |
| z | -0.1411 | -0.1644 | -0.1100 | 0.0614 | -0.2216 | 0.0805 | 0.0611 | -0.1952 | 0.1198 |
| Sn x | 0.0776 | -0.2022 | 0.1087 | 0.1240 | 0.2380 | -0.0300 | -0.0559 | 0.0439 | -0.1901 |
| y | 0.0017 | -0.1308 | 0.0437 | 0.0260 | -0.1274 | 0.0946 | -0.1407 | -0.2354 | 0.1877 |
| z | -0.0307 | -0.2042 | 0.2017 | 0.0304 | 0.1957 | -0.1399 | 0.0436 | -0.1665 | -0.0314 |
| Ag x | 0.2557 | -0.0710 | 0.3410 | 0.3789 | -0.1127 | -0.1438 | 0.2069 | 0.0871 | 0.1692 |
| y | -0.2110 | -0.3789 | -0.2513 | 0.0621 | 0.0550 | -0.1226 | -0.0659 | 0.0272 | 0.1195 |
| z | 0.0858 | 0.2047 | -0.0026 | 0.0589 | 0.0385 | 0.1820 | 0.0763 | 0.0137 | 0.0066 |

16: 46.2 17: 50.7 18: 53.5 19: 54.8 20: 57.9 21: 61.8 22: 62.2 23: 64.7 24: 66.6

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.0831 | 0.2032 | -0.0176 | -0.1572 | -0.0632 | 0.0884 | -0.4231 | -0.1761 | -0.0341 |
| y | 0.2349 | -0.0320 | -0.0786 | -0.0630 | 0.0391 | 0.2077 | -0.0528 | -0.0705 | 0.0151 |
| z | -0.0417 | -0.0810 | 0.0517 | 0.0034 | -0.1338 | -0.1578 | -0.2202 | -0.0302 | -0.0823 |
| Sn x | 0.1539 | -0.1421 | -0.0435 | -0.2916 | -0.0634 | -0.0198 | -0.0983 | 0.0340 | 0.2096 |
| y | -0.1576 | -0.0848 | -0.2949 | -0.2533 | 0.1613 | 0.0965 | -0.0159 | 0.0920 | -0.1722 |
| z | 0.2803 | 0.0644 | -0.0497 | 0.2430 | -0.0642 | 0.0652 | -0.1269 | 0.1143 | -0.0329 |
| Sn x | 0.0343 | 0.1092 | -0.0204 | -0.1048 | -0.2465 | -0.1520 | -0.0534 | -0.0858 | -0.1019 |
| y | 0.0575 | 0.1812 | 0.0532 | 0.0015 | 0.1379 | 0.0752 | 0.2596 | -0.1151 | 0.1815 |
| z | 0.0511 | -0.0906 | 0.0091 | -0.1068 | 0.1169 | 0.0775 | 0.0329 | -0.0212 | 0.0501 |
| Ag x | 0.2735 | -0.0296 | -0.0510 | -0.2222 | 0.0799 | 0.0418 | -0.0810 | -0.0597 | 0.0793 |
| y | -0.1742 | 0.0408 | -0.0292 | 0.1373 | -0.0298 | -0.0785 | 0.0723 | 0.1848 | 0.2138 |
| z | 0.0667 | 0.1333 | 0.1182 | 0.0242 | 0.1691 | 0.1117 | -0.1225 | -0.0576 | 0.0181 |
| Ag x | -0.1318 | 0.0166 | 0.1398 | -0.0520 | -0.2873 | 0.2808 | 0.1738 | 0.0937 | 0.0164 |
| y | 0.0124 | 0.0081 | 0.1062 | -0.0673 | 0.0123 | 0.3230 | 0.1360 | 0.0255 | 0.1334 |
| z | -0.1720 | 0.0047 | 0.0546 | 0.0300 | 0.0031 | 0.0528 | 0.1200 | 0.0296 | -0.0900 |
| Ag x | -0.1440 | -0.2828 | -0.0569 | 0.0938 | -0.0426 | 0.0300 | 0.0602 | 0.0390 | 0.0495 |
| y | -0.0273 | 0.2892 | 0.1528 | -0.2160 | 0.0333 | -0.0356 | 0.0525 | -0.0531 | -0.0284 |
| z | 0.3419 | 0.2856 | 0.1627 | 0.1966 | -0.1550 | -0.0258 | 0.0654 | -0.0481 | 0.0248 |
| Ag x | 0.0218 | -0.0234 | 0.0942 | 0.1349 | 0.0913 | -0.3316 | 0.0067 | -0.2627 | 0.0000 |
| y | -0.1476 | 0.0420 | -0.3395 | 0.0299 | 0.2436 | -0.2380 | -0.1841 | -0.0166 | 0.0967 |
| z | -0.2589 | -0.1583 | 0.2512 | -0.0777 | -0.0799 | 0.1641 | 0.1939 | -0.0690 | -0.0706 |
| Ag x | -0.1144 | -0.2260 | 0.0078 | 0.3533 | 0.0020 | 0.1607 | -0.2150 | 0.0019 | 0.2222 |
| y | -0.1019 | -0.2970 | -0.0972 | 0.2521 | -0.2916 | 0.1591 | 0.0185 | -0.1879 | -0.1179 |
| z | -0.1432 | 0.0549 | 0.0568 | -0.3214 | -0.1055 | -0.1780 | 0.0926 | -0.1257 | 0.2614 |
| Ag x | -0.1199 | 0.1985 | 0.0365 | 0.0558 | 0.0457 | -0.0679 | 0.0170 | 0.3157 | 0.2809 |
| y | 0.2513 | -0.2186 | 0.1206 | -0.1407 | -0.0067 | -0.2506 | 0.1997 | 0.0746 | -0.0267 |
| z | -0.0319 | 0.1178 | -0.2762 | 0.0739 | -0.0952 | -0.0264 | 0.0705 | 0.1969 | 0.0548 |
| Sn x | 0.1604 | -0.0646 | 0.1904 | -0.0124 | 0.0141 | 0.0946 | -0.0612 | 0.3504 | -0.2608 |
| y | -0.0557 | -0.0289 | -0.1252 | 0.1330 | -0.0156 | -0.0816 | 0.0430 | -0.2559 | 0.0173 |
| z | 0.0176 | 0.0704 | 0.1114 | 0.0363 | 0.0448 | -0.0753 | -0.1272 | 0.0623 | 0.1255 |
| Sn x | 0.0277 | -0.0721 | 0.2511 | 0.2028 | 0.1494 | -0.2030 | 0.0165 | -0.2014 | -0.0801 |
| y | 0.0589 | -0.1388 | 0.0543 | -0.0934 | -0.3016 | -0.1123 | -0.0984 | 0.0205 | 0.2754 |
| z | -0.0840 | 0.0911 | -0.2459 | 0.0858 | -0.2091 | -0.0422 | 0.0604 | 0.1053 | -0.0019 |
| Sn x | 0.1321 | 0.0064 | -0.2379 | 0.0484 | -0.1417 | -0.0324 | 0.1126 | -0.2834 | -0.1186 |
| y | 0.1466 | 0.0531 | -0.0995 | 0.0467 | 0.0075 | 0.0134 | -0.0573 | 0.1927 | -0.2518 |
| z | 0.0766 | -0.1647 | -0.0159 | -0.0958 | 0.1034 | 0.0581 | -0.1355 | 0.1538 | -0.0023 |
| Ag x | -0.1212 | 0.1135 | -0.0258 | 0.0302 | -0.0698 | -0.0258 | 0.0712 | 0.1464 | -0.0354 |
| y | -0.0984 | 0.3071 | 0.0192 | 0.1678 | 0.0216 | 0.1896 | -0.2618 | -0.1041 | 0.0511 |
| z | -0.2259 | 0.0579 | 0.0824 | -0.1449 | 0.0323 | 0.1901 | -0.1116 | -0.2382 | -0.2112 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.0704 | 0.0768 | -0.0682 | 0.1592 | 0.4121 | 0.1863 | 0.2742 | -0.0220 | -0.0890 |
| y | 0.1115 | -0.0474 | 0.1006 | -0.0305 | -0.0157 | 0.0637 | -0.1467 | -0.0084 | -0.1354 |
| z | 0.1268 | -0.1502 | -0.1034 | 0.1097 | 0.1428 | 0.0240 | 0.1258 | -0.0238 | 0.2952 |
| Sn x | -0.1165 | 0.2512 | -0.1658 | -0.0656 | -0.0648 | -0.0977 | 0.2945 | 0.0110 | -0.1479 |
| y | 0.0209 | 0.0013 | 0.1083 | 0.0613 | -0.1527 | -0.1941 | 0.0126 | 0.2411 | -0.2511 |
| z | 0.1566 | -0.1324 | -0.1933 | -0.0946 | 0.0148 | 0.0052 | 0.1697 | -0.1746 | -0.1170 |
| Ag x | -0.0617 | -0.1528 | -0.0272 | -0.1618 | 0.1850 | 0.0543 | -0.0979 | 0.1173 | 0.0404 |
| y | -0.1516 | -0.0709 | 0.3627 | 0.0442 | 0.1638 | -0.1408 | 0.0255 | -0.0242 | 0.0149 |
| z | -0.1887 | -0.0837 | 0.0076 | 0.0294 | 0.2147 | -0.2412 | -0.0764 | 0.1170 | -0.2330 |

25: 69.6 26: 73.2 27: 77.8 28: 80.7 29: 83.4 30: 89.2 31: 92.9 32: 93.5 33: 94.7

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.1645 | -0.0327 | 0.0754 | 0.0212 | 0.0865 | 0.2066 | -0.0014 | -0.0094 | -0.2227 |
| y | 0.1588 | -0.3285 | -0.0511 | -0.1763 | 0.1245 | -0.0130 | 0.3252 | -0.0960 | -0.0389 |
| z | -0.2135 | 0.3185 | 0.0402 | 0.0094 | -0.2241 | 0.0752 | -0.0952 | 0.1373 | -0.0898 |
| Sn x | 0.0565 | 0.0985 | 0.3221 | 0.0726 | -0.0983 | -0.1716 | 0.1055 | -0.1043 | -0.0564 |
| y | -0.0711 | -0.0646 | -0.3683 | 0.0695 | -0.0547 | 0.0451 | -0.0141 | 0.2236 | -0.0235 |
| z | 0.0716 | 0.0158 | -0.0087 | 0.0869 | 0.0791 | 0.0871 | 0.0221 | 0.1233 | -0.0442 |
| Sn x | 0.0204 | 0.0381 | -0.1564 | -0.3227 | -0.0841 | -0.2536 | 0.0129 | -0.1272 | -0.0911 |
| y | -0.2813 | -0.0501 | 0.1393 | -0.0513 | -0.0730 | -0.0333 | 0.1920 | 0.2119 | -0.0822 |
| z | 0.0104 | -0.0407 | -0.0614 | 0.1105 | -0.0632 | 0.0907 | -0.0325 | -0.0310 | 0.0228 |
| Ag x | 0.0161 | -0.0626 | -0.0689 | 0.0440 | 0.0998 | -0.1136 | -0.1698 | -0.1100 | 0.3514 |
| y | -0.0617 | 0.0359 | -0.1550 | -0.1184 | 0.0513 | 0.1527 | -0.2003 | -0.2252 | 0.1086 |
| z | 0.1398 | 0.1579 | -0.0488 | -0.0275 | -0.1337 | 0.0526 | -0.0112 | -0.1372 | 0.0206 |
| Ag x | 0.0874 | -0.0073 | -0.0761 | -0.0585 | 0.1299 | -0.0524 | 0.1537 | 0.0128 | -0.0212 |
| y | 0.0018 | 0.0223 | -0.0330 | 0.0276 | 0.0139 | 0.0135 | -0.2359 | -0.1275 | -0.1324 |
| z | -0.0385 | 0.0693 | 0.0276 | -0.0021 | 0.0322 | -0.0329 | 0.1908 | -0.1584 | 0.1260 |
| Ag x | -0.0417 | 0.0042 | -0.0588 | -0.0436 | 0.0495 | 0.3809 | 0.0835 | -0.2091 | -0.1326 |
| y | 0.0716 | -0.0039 | -0.0261 | 0.1531 | 0.1333 | -0.0562 | -0.2425 | 0.1067 | 0.2900 |
| z | 0.0205 | -0.0472 | 0.1123 | 0.0340 | -0.0077 | -0.0716 | 0.0097 | -0.0472 | 0.0619 |
| Ag x | 0.0171 | -0.2921 | -0.0212 | 0.0970 | -0.0853 | 0.0248 | -0.0385 | -0.1249 | -0.0621 |
| y | 0.1719 | -0.0805 | 0.1502 | -0.1560 | -0.0074 | 0.0213 | -0.0381 | 0.1915 | 0.0813 |
| z | 0.1326 | 0.0591 | -0.1512 | -0.1019 | 0.1044 | -0.0520 | -0.0078 | 0.0351 | -0.0691 |
| Ag x | 0.2073 | 0.1663 | 0.1519 | -0.1652 | 0.2821 | -0.0580 | -0.0975 | 0.3234 | 0.2444 |
| y | 0.0206 | -0.3173 | 0.2160 | 0.0715 | -0.3441 | -0.1229 | -0.2471 | -0.0884 | 0.0809 |
| z | 0.3252 | -0.1588 | 0.1530 | -0.2164 | -0.1076 | 0.2759 | -0.1741 | 0.0938 | -0.1708 |
| Ag x | 0.1008 | -0.0026 | -0.2857 | 0.0107 | -0.3809 | -0.2022 | 0.0584 | -0.0231 | 0.1492 |
| y | 0.2071 | 0.1408 | 0.0106 | -0.0173 | 0.0520 | -0.0312 | 0.1551 | 0.2017 | -0.1157 |
| z | -0.0086 | 0.1005 | 0.0161 | 0.0315 | 0.1431 | -0.0391 | 0.0449 | 0.0583 | 0.0878 |
| Sn x | -0.1606 | -0.2016 | 0.0585 | -0.2452 | -0.1166 | 0.0929 | -0.0153 | 0.3993 | -0.0102 |
| y | 0.1520 | 0.3245 | -0.0874 | 0.1714 | 0.0647 | -0.2647 | 0.1279 | 0.0449 | -0.2300 |
| z | -0.0593 | -0.0031 | -0.1325 | -0.0712 | 0.1158 | 0.1496 | -0.1315 | -0.1088 | 0.0069 |
| Sn x | -0.0217 | -0.0898 | -0.3413 | 0.0905 | 0.2196 | -0.1063 | -0.1227 | 0.1117 | -0.2029 |
| y | -0.2597 | -0.0901 | -0.0200 | 0.0972 | 0.2289 | 0.0167 | 0.1206 | -0.0905 | 0.1759 |
| z | -0.1144 | -0.0970 | 0.0101 | 0.1219 | -0.0929 | -0.0745 | 0.0774 | 0.0163 | -0.0835 |
| Sn x | -0.0267 | 0.1135 | -0.2488 | 0.1108 | -0.1167 | 0.3165 | 0.1403 | 0.0394 | 0.3410 |
| y | -0.1558 | 0.0014 | -0.0035 | -0.1315 | 0.1589 | -0.1029 | -0.3118 | -0.2354 | -0.1618 |
| z | 0.1231 | -0.1567 | -0.1182 | 0.3775 | -0.0249 | 0.0970 | 0.1049 | 0.0182 | -0.0772 |
| Ag x | 0.0228 | -0.0898 | 0.0380 | 0.1423 | -0.1810 | -0.1673 | 0.0524 | 0.1035 | -0.0832 |
| y | 0.0218 | 0.0006 | -0.0121 | -0.0777 | -0.0074 | 0.0769 | 0.2871 | -0.0231 | -0.1731 |
| z | -0.0074 | -0.0941 | 0.1073 | 0.1716 | 0.0565 | -0.1964 | -0.0552 | 0.1249 | 0.1932 |
| Sn x | 0.1403 | 0.0756 | 0.2154 | 0.0229 | -0.1151 | 0.1594 | -0.0345 | -0.1661 | 0.0000 |
| y | 0.1172 | 0.2959 | -0.0781 | -0.1470 | -0.2987 | -0.0212 | -0.1389 | -0.0555 | 0.0066 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| z | -0.2473 | -0.1017 | -0.0234 | 0.0285 | -0.0023 | -0.1592 | -0.1980 | 0.1271 | -0.2037 |
| Sn x | -0.1027 | 0.0504 | 0.2161 | 0.0383 | 0.2502 | 0.0753 | -0.1438 | 0.0668 | -0.0841 |
| y | 0.2638 | 0.0421 | 0.1831 | 0.2691 | 0.0794 | 0.2139 | 0.0102 | -0.0570 | 0.0113 |
| z | -0.1547 | 0.1633 | 0.0128 | -0.3485 | 0.0012 | 0.0132 | 0.0570 | -0.0136 | 0.1219 |
| Ag x | -0.1382 | 0.2291 | 0.1730 | 0.1954 | 0.0592 | -0.1469 | 0.0199 | -0.1932 | -0.1036 |
| y | -0.3531 | 0.0651 | 0.1494 | 0.0110 | -0.1328 | 0.1130 | 0.1953 | 0.0209 | 0.2198 |
| z | 0.0492 | -0.1900 | 0.0786 | -0.2195 | 0.1345 | -0.2293 | 0.2083 | -0.2512 | 0.1142 |

34: 99.8 35: 104.9 36: 106.7 37: 112.1 38: 118.1 39: 120.4 40: 126.2 41: 128.4 42: 129.4

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.1436 | 0.3417 | 0.0210 | 0.1308 | -0.0920 | -0.0027 | -0.0917 | 0.0963 | 0.0578 |
| y | 0.1044 | 0.2734 | -0.0849 | 0.0521 | -0.0894 | 0.0242 | 0.0421 | -0.2142 | 0.0657 |
| z | 0.0009 | 0.0239 | 0.1163 | -0.0106 | -0.0314 | -0.0370 | 0.0098 | 0.0042 | -0.1525 |
| Sn x | 0.1520 | 0.0575 | -0.1279 | -0.2159 | 0.0260 | -0.2525 | -0.0134 | 0.0899 | 0.0477 |
| y | 0.1648 | -0.0759 | 0.0728 | 0.0360 | -0.0737 | -0.2931 | 0.3152 | -0.0506 | 0.1537 |
| z | 0.0589 | -0.1153 | -0.0267 | 0.0094 | -0.0114 | 0.0183 | 0.1330 | -0.0606 | 0.1649 |
| Sn x | 0.1198 | -0.1772 | -0.1073 | 0.3602 | 0.2247 | 0.0766 | -0.0570 | -0.0360 | 0.0865 |
| y | 0.2778 | -0.1793 | 0.1869 | 0.0116 | -0.0812 | 0.2753 | -0.0731 | 0.0650 | -0.1252 |
| z | -0.0378 | 0.0615 | 0.0349 | 0.1197 | 0.2451 | 0.0536 | -0.2366 | 0.0105 | -0.0511 |
| Ag x | -0.0155 | -0.3755 | -0.0028 | -0.2723 | 0.2032 | 0.0997 | 0.0388 | 0.0584 | 0.0329 |
| y | 0.2689 | -0.0495 | -0.0815 | -0.1591 | -0.0092 | 0.1493 | -0.0228 | 0.0496 | 0.1582 |
| z | 0.0078 | -0.0814 | 0.0316 | 0.0668 | -0.3964 | 0.0265 | -0.2194 | 0.1113 | 0.4006 |
| Ag x | 0.1008 | -0.0093 | 0.0984 | -0.1922 | -0.2137 | 0.1609 | 0.0147 | 0.0522 | -0.1796 |
| y | -0.1023 | 0.0422 | -0.1662 | 0.3034 | 0.2416 | -0.2099 | -0.0902 | 0.2262 | 0.0238 |
| z | -0.0311 | 0.0300 | -0.0514 | 0.0725 | 0.1890 | -0.0236 | 0.0912 | -0.4104 | 0.3403 |
| Ag x | -0.3139 | 0.0078 | -0.0102 | -0.3017 | -0.1058 | -0.0972 | 0.0520 | -0.0114 | 0.0068 |
| y | -0.2419 | 0.3126 | -0.0017 | -0.0980 | -0.1553 | 0.0617 | 0.0655 | -0.1009 | -0.0377 |
| z | 0.0169 | 0.1142 | -0.0214 | -0.1923 | -0.0825 | -0.3373 | 0.1246 | 0.0730 | 0.0023 |
| Ag x | -0.0960 | -0.0713 | 0.1122 | 0.1911 | -0.1458 | 0.0898 | 0.1316 | 0.0747 | -0.0684 |
| y | 0.0536 | 0.0329 | -0.0812 | -0.1224 | 0.0393 | -0.1642 | -0.1763 | 0.2085 | -0.0773 |
| z | 0.0519 | 0.0023 | -0.0824 | -0.0162 | -0.0194 | -0.1448 | -0.1131 | 0.3173 | -0.1441 |
| Ag x | -0.0202 | 0.0561 | 0.0866 | 0.2545 | 0.0158 | 0.1302 | 0.1852 | -0.0073 | 0.0309 |
| y | 0.1427 | 0.0203 | 0.0781 | -0.0971 | -0.0376 | -0.0251 | -0.1218 | -0.1374 | 0.0485 |
| z | -0.1380 | -0.1059 | 0.1248 | -0.0170 | 0.0335 | 0.0786 | 0.0440 | -0.2750 | 0.0852 |
| Ag x | -0.0966 | 0.1762 | 0.2609 | 0.0018 | -0.0129 | -0.0056 | -0.0809 | 0.0855 | 0.0779 |
| y | -0.1685 | 0.1021 | 0.0507 | 0.0863 | 0.0589 | 0.0163 | 0.1056 | 0.0419 | -0.0185 |
| z | 0.0011 | -0.1345 | 0.0406 | 0.1310 | -0.1670 | -0.2745 | -0.3537 | -0.3012 | -0.2096 |
| Sn x | -0.1020 | 0.0295 | -0.1105 | -0.1413 | 0.0954 | 0.0655 | -0.2208 | 0.0074 | 0.1636 |
| y | -0.0193 | 0.1668 | -0.0904 | -0.2385 | 0.1070 | 0.2292 | -0.1905 | -0.0671 | 0.1250 |
| z | 0.3421 | 0.2089 | -0.1244 | -0.1407 | 0.2981 | 0.0870 | 0.1537 | -0.1476 | -0.3253 |
| Sn x | 0.1577 | -0.0720 | 0.1580 | -0.1193 | 0.0084 | -0.2804 | -0.0534 | -0.1125 | 0.0869 |
| y | -0.1008 | -0.1064 | 0.1072 | 0.2565 | -0.1525 | -0.1593 | 0.0137 | 0.0507 | -0.0525 |
| z | -0.0916 | 0.1411 | 0.0455 | -0.0027 | 0.1475 | 0.1460 | 0.4154 | 0.3415 | 0.1596 |
| Sn x | -0.1292 | 0.1061 | -0.2318 | 0.0673 | 0.0642 | 0.0885 | -0.1781 | 0.0451 | -0.0922 |
| y | -0.2815 | 0.1001 | 0.2616 | -0.0058 | 0.0102 | 0.1675 | -0.1173 | -0.0685 | -0.1200 |
| z | 0.0883 | -0.1294 | -0.0081 | 0.0637 | -0.1136 | 0.3222 | -0.0872 | 0.0116 | -0.1551 |
| Ag x | -0.0252 | 0.0267 | -0.1304 | 0.0429 | 0.0396 | -0.0900 | 0.0432 | -0.2324 | -0.2938 |
| y | -0.3263 | -0.3832 | 0.0395 | -0.1588 | 0.2295 | -0.0878 | 0.0442 | 0.0190 | -0.1157 |
| z | -0.0909 | -0.0899 | 0.0666 | -0.0372 | 0.0936 | 0.0109 | 0.0343 | 0.0396 | -0.0148 |
| Sn x | 0.0614 | 0.0548 | 0.1206 | 0.1794 | 0.0599 | -0.1116 | 0.1459 | 0.0094 | -0.1710 |
| y | 0.0229 | -0.1623 | -0.2797 | 0.0266 | -0.3052 | 0.0523 | 0.2909 | -0.0839 | -0.2082 |
| z | -0.1894 | -0.0164 | -0.3413 | 0.0324 | -0.0829 | 0.0366 | -0.0168 | 0.0134 | 0.0504 |
| Sn x | 0.0589 | -0.1529 | -0.2469 | 0.0101 | -0.1718 | 0.0802 | 0.0557 | 0.0243 | 0.1462 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| y | 0.1878 | -0.1166 | 0.1090 | 0.0720 | 0.1668 | -0.0254 | -0.0962 | 0.1660 | 0.0918 |
| z | 0.0643 | 0.0640 | 0.3928 | -0.0861 | 0.0172 | -0.0396 | 0.0130 | 0.0906 | -0.0165 |
| Ag x | -0.0183 | -0.0072 | 0.1358 | -0.0083 | -0.0057 | 0.0650 | 0.0484 | -0.1497 | 0.0518 |
| y | 0.0005 | 0.0278 | -0.1342 | 0.0248 | 0.0710 | -0.0243 | 0.0022 | -0.0944 | 0.0917 |
| z | -0.0651 | 0.0152 | -0.2016 | 0.0080 | -0.1423 | 0.0484 | -0.0110 | 0.1691 | -0.1184 |

43: 135.8 44: 139.3 45: 143.7 46: 147.7 47: 151.2 48: 173.5

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|---|---|---|---|---|---|---|
| Sn x | 0.0024 | -0.0603 | -0.0436 | -0.0545 | -0.0373 | -0.3012 |
| y | -0.0609 | 0.0891 | 0.0336 | 0.0033 | 0.1026 | 0.3517 |
| z | 0.0148 | 0.0120 | 0.0596 | 0.0679 | -0.0063 | 0.6107 |
| Sn x | -0.0674 | -0.0212 | 0.0776 | -0.0003 | 0.0465 | -0.0083 |
| y | 0.3471 | -0.1011 | 0.0617 | -0.0882 | -0.0085 | 0.0007 |
| z | -0.3706 | -0.3386 | 0.4185 | 0.0878 | -0.0093 | -0.0176 |
| Sn x | -0.0941 | -0.0271 | -0.0822 | 0.0685 | -0.0025 | 0.0256 |
| y | -0.0599 | 0.0091 | 0.0115 | -0.0084 | -0.0264 | -0.0112 |
| z | 0.0970 | 0.2929 | 0.4748 | -0.4117 | 0.0526 | -0.0264 |
| Ag x | 0.0703 | 0.0181 | 0.0399 | 0.0829 | -0.0057 | 0.0735 |
| y | 0.1194 | 0.0904 | 0.0908 | 0.1655 | -0.0501 | 0.0446 |
| z | 0.1002 | 0.1901 | 0.1101 | 0.1766 | -0.1086 | 0.0272 |
| Ag x | 0.0279 | 0.0475 | 0.1285 | -0.1706 | -0.0787 | -0.0310 |
| y | 0.0182 | -0.2505 | -0.1088 | 0.1377 | -0.2372 | 0.1510 |
| z | -0.0865 | 0.1472 | -0.1411 | 0.1065 | 0.2858 | -0.1281 |
| Ag x | -0.0985 | -0.1064 | -0.0195 | 0.0543 | 0.0049 | 0.0096 |
| y | -0.2076 | -0.1124 | 0.0991 | 0.2010 | -0.0611 | -0.0246 |
| z | 0.4004 | 0.1255 | -0.2651 | -0.0935 | 0.0300 | 0.0163 |
| Ag x | 0.2659 | -0.2269 | 0.1982 | 0.1515 | 0.4035 | -0.0276 |
| y | -0.2239 | 0.2359 | -0.0641 | 0.1019 | 0.2019 | -0.0149 |
| z | -0.0645 | 0.0813 | 0.0536 | 0.1938 | 0.3952 | -0.0206 |
| Ag x | 0.2015 | 0.0756 | -0.0665 | -0.0259 | -0.0517 | 0.0093 |
| y | -0.0856 | -0.0882 | -0.0416 | -0.0783 | -0.0502 | 0.0111 |
| z | 0.0694 | 0.0098 | -0.0603 | -0.0851 | -0.2092 | 0.0033 |
| Ag x | -0.1376 | -0.2144 | -0.1371 | -0.2454 | 0.1258 | 0.0270 |
| y | -0.0333 | 0.0025 | -0.0359 | -0.0523 | 0.0046 | -0.0053 |
| z | 0.0209 | -0.1670 | -0.0189 | -0.0489 | 0.0509 | -0.0262 |
| Sn x | 0.1214 | -0.0736 | -0.0246 | 0.0790 | 0.0891 | 0.0044 |
| y | 0.2450 | -0.2056 | 0.0374 | 0.0296 | -0.0053 | 0.0193 |
| z | 0.0302 | -0.1663 | -0.0441 | -0.0479 | 0.0964 | -0.0239 |
| Sn x | -0.3014 | 0.2274 | -0.0961 | -0.1018 | -0.2588 | 0.0212 |
| y | -0.0567 | 0.0787 | 0.0318 | 0.0147 | 0.0225 | 0.0050 |
| z | -0.1501 | 0.2546 | 0.0046 | 0.0228 | -0.1038 | 0.0147 |
| Sn x | 0.0050 | 0.0948 | -0.0818 | -0.0754 | -0.1202 | -0.0023 |
| y | 0.0466 | 0.2204 | -0.0348 | -0.0449 | 0.1124 | -0.0046 |
| z | -0.0362 | 0.0214 | -0.4872 | 0.1995 | -0.0241 | 0.0379 |
| Ag x | 0.1462 | 0.2589 | 0.2497 | 0.4642 | -0.2401 | -0.1440 |
| y | 0.0226 | -0.0199 | -0.0222 | -0.0310 | 0.0058 | -0.0309 |
| z | -0.0624 | -0.0923 | -0.0643 | -0.1162 | 0.0562 | 0.0282 |
| Sn x | -0.0916 | 0.0024 | -0.0192 | 0.0012 | -0.0233 | 0.1079 |
| y | -0.1456 | 0.0928 | -0.0418 | -0.2071 | 0.0830 | -0.2404 |
| z | -0.0014 | -0.0231 | -0.0549 | -0.1139 | 0.0160 | -0.2602 |
| Sn x | -0.0458 | -0.0358 | -0.0857 | -0.1957 | 0.1412 | 0.2352 |
| y | 0.0601 | -0.0369 | -0.0015 | -0.0873 | -0.0277 | -0.2307 |
| z | -0.0125 | -0.1604 | -0.0677 | 0.2203 | -0.1183 | -0.2901 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Ag x | 0.0190 | 0.0360 | -0.0201 | -0.0181 | 0.0155 | -0.0033 |
| y | -0.0040 | -0.0116 | -0.0196 | -0.0374 | -0.0786 | -0.0156 |
| z | 0.0722 | -0.1819 | 0.0676 | -0.1592 | -0.3989 | 0.0524 |