$coordinates

| | | | |
|---|---|---|---|
| Sn | 3.51268507234061 | 2.80327997828436 | 3.24373221100171 |
| Sn | -3.46368431707226 | -4.27029861997224 | 3.74781335916138 |
| Sn | 5.81701065574308 | -0.74310907192226 | -1.21124453381317 |
| Ag | 1.97420398626131 | -3.63120424837464 | -4.00269489458521 |
| Ag | -1.04979229388992 | 5.05165369075263 | 0.44911266235504 |
| Ag | -6.34410646846397 | 3.04860147616924 | -4.54281097888881 |
| Ag | -9.77578095470018 | -0.03838958780800 | -1.02105582775032 |
| Ag | -0.80531554326716 | 4.39013478582702 | -5.03478828759872 |
| Ag | 0.77193992421262 | -1.65906492207544 | 0.96154569322961 |
| Sn | 3.88972105183483 | 5.23355453991142 | -2.24721743440581 |
| Sn | -2.13270299621149 | 1.58258098971030 | 4.64568570192857 |
| Sn | -7.57869921294804 | -2.17271485342656 | -5.89181889425386 |
| Sn | 2.99068562421169 | 0.90435756724390 | -7.06495320414127 |
| Ag | -2.32548167397386 | -0.87513011057278 | -5.94782467907441 |
| Ag | -6.57806729382308 | 4.32287247695664 | 0.82961756485376 |
| Sn | -7.71799915726832 | 1.18057722677728 | 5.07296448564296 |
| Ag | -4.42870726888831 | -0.66795961690344 | -0.54817358170330 |
| Sn | -3.06104648299416 | -5.72310712213308 | -2.56315331861982 |
| Ag | -4.53024326269796 | 7.87239795663551 | -2.74633610317975 |
| Sn | 8.00928678238538 | 2.79282754025960 | -5.16541925693978 |
| Sn | -8.60164775637009 | -5.90802963391711 | -1.42563102039012 |
| Ag | -8.94191044403910 | -3.81794619414098 | 3.49084716858332 |

$end

vibrational frequencies, intensities

| mode | au_amu | cm-1 | km/mol |
|---|---|---|---|
| 7 | 0.003556 | 18.3 | 0.24 |
| 8 | 0.004301 | 22.1 | 0.01 |
| 9 | 0.004498 | 23.1 | 0.05 |
| 10 | 0.004987 | 25.6 | 0.11 |
| 11 | 0.005543 | 28.5 | 0.08 |
| 12 | 0.005951 | 30.6 | 0.11 |
| 13 | 0.006116 | 31.4 | 0.02 |
| 14 | 0.006413 | 33.0 | 0.12 |
| 15 | 0.006822 | 35.1 | 0.03 |
| 16 | 0.007062 | 36.3 | 0.04 |
| 17 | 0.007530 | 38.7 | 0.01 |
| 18 | 0.007845 | 40.3 | 0.21 |
| 19 | 0.008189 | 42.1 | 0.09 |
| 20 | 0.008760 | 45.0 | 0.04 |
| 21 | 0.008987 | 46.2 | 0.04 |
| 22 | 0.009349 | 48.1 | 0.13 |
| 23 | 0.009434 | 48.5 | 0.07 |
| 24 | 0.009841 | 50.6 | 0.25 |
| 25 | 0.010066 | 51.7 | 0.04 |
| 26 | 0.010357 | 53.2 | 0.11 |
| 27 | 0.010690 | 55.0 | 0.03 |
| 28 | 0.011116 | 57.1 | 0.08 |
| 29 | 0.011325 | 58.2 | 0.05 |
| 30 | 0.011684 | 60.1 | 0.16 |

| | | | |
|---|---|---|---|
| 31 | 0.012330 | 63.4 | 0.23 |
| 32 | 0.012764 | 65.6 | 0.01 |
| 33 | 0.013274 | 68.2 | 0.05 |
| 34 | 0.013655 | 70.2 | 0.29 |
| 35 | 0.014095 | 72.5 | 0.19 |
| 36 | 0.014378 | 73.9 | 0.10 |
| 37 | 0.014636 | 75.2 | 0.18 |
| 38 | 0.015474 | 79.5 | 0.49 |
| 39 | 0.016071 | 82.6 | 0.14 |
| 40 | 0.016259 | 83.6 | 0.08 |
| 41 | 0.016829 | 86.5 | 0.23 |
| 42 | 0.017492 | 89.9 | 0.03 |
| 43 | 0.017817 | 91.6 | 0.02 |
| 44 | 0.018031 | 92.7 | 0.06 |
| 45 | 0.018725 | 96.3 | 0.10 |
| 46 | 0.019446 | 100.0 | 0.26 |
| 47 | 0.019975 | 102.7 | 0.09 |
| 48 | 0.020693 | 106.4 | 0.09 |
| 49 | 0.020996 | 107.9 | 0.19 |
| 50 | 0.021386 | 109.9 | 0.14 |
| 51 | 0.022126 | 113.7 | 0.20 |
| 52 | 0.022449 | 115.4 | 0.82 |
| 53 | 0.022511 | 115.7 | 0.13 |
| 54 | 0.023132 | 118.9 | 0.10 |
| 55 | 0.023370 | 120.1 | 0.18 |
| 56 | 0.023670 | 121.7 | 0.07 |
| 57 | 0.024540 | 126.1 | 0.02 |
| 58 | 0.025241 | 129.8 | 0.06 |
| 59 | 0.025960 | 133.4 | 0.35 |
| 60 | 0.026370 | 135.6 | 0.23 |
| 61 | 0.028052 | 144.2 | 0.21 |
| 62 | 0.028126 | 144.6 | 0.17 |
| 63 | 0.028605 | 147.0 | 0.63 |
| 64 | 0.029160 | 149.9 | 0.15 |
| 65 | 0.030001 | 154.2 | 0.17 |
| 66 | 0.031244 | 160.6 | 2.93 |

Frequencies (cm-1) and normal modes

| | 7: 18.3 | 8: 22.1 | 9: 23.1 | 10: 25.6 | 11: 28.5 | 12: 30.6 | 13: 31.4 | 14: 33.0 | 15: 35.1 |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.0008 | 0.0933 | -0.0658 | -0.0311 | -0.0040 | 0.0783 | -0.0393 | 0.0986 | 0.1425 |
| y | -0.2206 | 0.0709 | 0.0354 | 0.2655 | -0.0807 | 0.0313 | -0.0133 | -0.1619 | -0.2144 |
| z | -0.0235 | 0.1063 | 0.0514 | -0.0472 | -0.0034 | -0.0862 | 0.0411 | 0.0268 | 0.0336 |
| Sn x | -0.1867 | 0.0322 | 0.1791 | -0.1572 | -0.2774 | -0.0981 | -0.0082 | 0.0969 | 0.0230 |
| y | -0.0515 | -0.1223 | -0.1655 | -0.1539 | -0.0196 | -0.0240 | -0.0550 | 0.3171 | 0.0153 |
| z | 0.0669 | -0.2344 | -0.2725 | -0.0748 | -0.1447 | -0.0421 | -0.0924 | 0.2462 | 0.2691 |
| Sn x | -0.0234 | 0.0564 | 0.1085 | -0.0651 | 0.0383 | 0.1627 | -0.0058 | 0.0336 | -0.1014 |
| y | -0.0665 | -0.0152 | -0.0516 | 0.1452 | 0.0667 | 0.1807 | 0.1426 | -0.1998 | 0.1829 |
| z | -0.1076 | 0.0344 | -0.0256 | 0.1012 | -0.0140 | -0.0470 | 0.1176 | -0.0984 | -0.1497 |
| Ag x | 0.0855 | -0.0663 | 0.0286 | -0.1174 | 0.0793 | 0.2443 | 0.1080 | -0.0509 | -0.1799 |
| y | 0.0410 | -0.0552 | -0.0637 | 0.1128 | 0.0788 | -0.1786 | 0.1084 | -0.0194 | 0.0331 |
| z | -0.2551 | 0.1173 | -0.0252 | 0.2282 | -0.0108 | 0.1654 | -0.1006 | -0.0792 | 0.0735 |
| Ag x | -0.1114 | -0.0033 | -0.2124 | -0.0752 | 0.0766 | -0.0356 | 0.0724 | -0.1381 | 0.1177 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| y | -0.1348 | 0.3590 | -0.2728 | -0.3542 | 0.1355 | -0.1798 | -0.1307 | -0.1830 | -0.0869 |
| z | -0.0018 | 0.2516 | -0.0019 | -0.1977 | 0.1278 | 0.1081 | -0.1023 | -0.0579 | 0.0482 |
| Ag x | 0.0080 | -0.0916 | 0.0663 | 0.0583 | -0.0906 | 0.0049 | -0.0236 | -0.1660 | 0.1516 |
| y | -0.0426 | -0.0642 | 0.0508 | 0.0018 | 0.0506 | 0.0499 | -0.0884 | 0.0255 | -0.0167 |
| z | -0.0489 | -0.1090 | -0.1429 | 0.0537 | -0.0297 | 0.0755 | 0.0746 | -0.0087 | -0.1834 |
| Ag x | -0.0378 | 0.0872 | 0.0105 | 0.1559 | 0.1762 | -0.0755 | -0.1371 | 0.1313 | 0.0020 |
| y | -0.0596 | -0.0860 | -0.0226 | -0.0620 | 0.0250 | 0.1287 | 0.1301 | -0.0604 | 0.1222 |
| z | -0.1578 | -0.1575 | 0.0332 | -0.0326 | 0.3082 | -0.1079 | 0.1724 | 0.0661 | -0.1749 |
| Ag x | 0.0060 | -0.1195 | 0.0686 | -0.0001 | -0.0496 | -0.0878 | 0.0428 | -0.1432 | 0.1046 |
| y | 0.1380 | -0.1783 | 0.0158 | 0.1139 | -0.1562 | -0.2147 | -0.2785 | -0.2118 | -0.0012 |
| z | -0.0219 | 0.2745 | -0.0267 | -0.2408 | 0.0940 | 0.0725 | -0.1435 | -0.0507 | -0.0112 |
| Ag x | -0.0201 | 0.1349 | 0.0736 | 0.1366 | 0.0667 | -0.0368 | -0.1247 | 0.1141 | -0.0090 |
| y | -0.2775 | 0.0236 | 0.1355 | -0.1729 | -0.1835 | 0.1603 | 0.0710 | -0.0800 | -0.1730 |
| z | -0.0863 | 0.0432 | -0.1345 | 0.3662 | 0.1235 | -0.1045 | -0.1954 | 0.0696 | 0.1535 |
| Sn x | -0.0448 | -0.0926 | -0.0340 | -0.0390 | -0.0441 | -0.1100 | -0.0790 | -0.2223 | -0.0452 |
| y | -0.0115 | -0.0124 | -0.0990 | 0.1349 | 0.0068 | 0.0317 | 0.1568 | -0.1761 | 0.2593 |
| z | 0.0930 | 0.0861 | 0.1241 | -0.1607 | -0.0018 | -0.1218 | -0.0168 | 0.1055 | 0.1370 |
| Sn x | 0.1229 | 0.1776 | -0.0197 | 0.1114 | -0.0646 | 0.0723 | -0.0005 | 0.0581 | 0.0493 |
| y | -0.1844 | -0.0911 | -0.1923 | -0.1393 | -0.0646 | -0.1477 | -0.0891 | 0.1661 | 0.0095 |
| z | -0.0108 | -0.0956 | 0.1195 | 0.0908 | 0.0031 | 0.1697 | -0.0431 | 0.1127 | 0.0572 |
| Sn x | 0.1286 | -0.0404 | 0.0052 | 0.0038 | -0.0657 | 0.0897 | -0.2405 | -0.0541 | -0.0377 |
| y | -0.1753 | -0.1232 | 0.0292 | 0.0700 | 0.0018 | 0.0981 | 0.0252 | 0.1253 | -0.0389 |
| z | 0.0787 | -0.1265 | 0.0454 | -0.0808 | 0.1704 | -0.0654 | 0.0843 | -0.1258 | -0.0501 |
| Sn x | 0.0135 | -0.0766 | 0.0613 | 0.0085 | -0.0251 | -0.0399 | 0.2489 | 0.0816 | -0.0536 |
| y | 0.1686 | -0.0269 | -0.0486 | -0.0559 | 0.0179 | -0.1738 | 0.0019 | -0.0175 | 0.0243 |
| z | -0.0854 | 0.1363 | 0.0151 | -0.0030 | -0.0547 | 0.0114 | -0.0368 | -0.0125 | -0.0053 |
| Ag x | 0.0430 | -0.0451 | 0.0441 | -0.0021 | -0.0320 | 0.1282 | -0.0853 | -0.0575 | -0.0729 |
| y | 0.1233 | -0.1050 | 0.0224 | 0.0477 | -0.0896 | -0.2463 | -0.1811 | -0.1114 | -0.0117 |
| z | 0.1082 | -0.1117 | 0.0837 | -0.1414 | -0.1356 | 0.1761 | -0.1391 | -0.2034 | 0.0131 |
| Ag x | -0.1777 | -0.0061 | -0.2707 | -0.0638 | 0.1400 | -0.0713 | 0.1358 | -0.1345 | 0.1503 |
| y | 0.0492 | -0.0459 | 0.1298 | -0.0556 | 0.1477 | 0.0795 | -0.0126 | 0.0397 | -0.0892 |
| z | -0.0878 | -0.0873 | -0.1826 | 0.0698 | -0.0546 | 0.0971 | 0.0960 | 0.0322 | -0.2074 |
| Sn x | 0.1483 | 0.2541 | -0.0882 | 0.1284 | -0.1310 | 0.0143 | 0.0331 | 0.0368 | 0.0205 |
| y | 0.2550 | 0.1864 | 0.0869 | -0.0085 | -0.0641 | -0.0194 | 0.0943 | -0.0168 | -0.0077 |
| z | 0.0991 | 0.1150 | -0.2122 | 0.1466 | -0.2940 | 0.0147 | 0.1763 | 0.0543 | -0.1802 |
| Ag x | -0.0394 | 0.1281 | 0.0440 | 0.2318 | 0.2501 | -0.1085 | -0.1737 | 0.2130 | -0.0500 |
| y | 0.0791 | 0.0247 | 0.1761 | 0.0439 | 0.1760 | 0.0594 | -0.1141 | 0.1786 | -0.2369 |
| z | 0.0900 | -0.0914 | 0.0190 | -0.0135 | -0.1645 | 0.0700 | -0.0386 | -0.0244 | 0.0975 |
| Sn x | 0.1472 | -0.1746 | -0.1261 | -0.0947 | 0.1116 | 0.0534 | -0.0330 | 0.0305 | -0.1106 |
| y | 0.0756 | -0.0612 | 0.0428 | -0.0102 | 0.0209 | 0.0028 | 0.0282 | 0.1248 | -0.1612 |
| z | 0.1462 | -0.1667 | -0.0331 | -0.1213 | 0.0297 | 0.1782 | -0.2376 | 0.0764 | 0.0312 |
| Ag x | -0.0475 | -0.0911 | 0.0603 | -0.0103 | 0.1271 | 0.1251 | 0.1462 | -0.0327 | 0.1783 |
| y | 0.0009 | -0.0202 | 0.0247 | -0.0232 | 0.0437 | -0.0105 | -0.1519 | -0.0543 | -0.0358 |
| z | -0.0211 | -0.0437 | -0.0451 | 0.0703 | -0.0854 | 0.1343 | -0.1016 | -0.0558 | -0.0550 |
| Sn x | -0.0048 | -0.0792 | -0.0055 | 0.0018 | -0.0564 | -0.1163 | 0.1312 | -0.0229 | -0.1591 |
| y | 0.0924 | 0.0791 | 0.1012 | -0.0807 | 0.1071 | 0.2033 | 0.2007 | 0.1916 | 0.3506 |
| z | 0.0662 | 0.0454 | 0.0112 | -0.0026 | -0.0859 | -0.2787 | 0.3078 | 0.2159 | -0.0500 |
| Sn x | 0.1631 | -0.1429 | -0.1104 | -0.0358 | 0.1471 | -0.0364 | 0.0332 | -0.0029 | -0.1349 |
| y | -0.1505 | 0.0053 | 0.1934 | 0.0725 | -0.0832 | 0.0558 | -0.0187 | 0.1209 | 0.1281 |
| z | 0.1742 | 0.0394 | 0.2179 | -0.0090 | 0.1304 | -0.1790 | 0.1062 | -0.1905 | 0.0426 |
| Ag x | -0.1942 | 0.0654 | 0.1873 | -0.1364 | -0.3541 | -0.1606 | -0.0030 | 0.1241 | 0.0345 |
| y | 0.3650 | 0.2635 | -0.1245 | 0.0964 | -0.1325 | 0.1018 | 0.1509 | -0.0204 | -0.0786 |
| z | -0.0389 | -0.0227 | 0.3796 | 0.0065 | 0.1050 | -0.2183 | 0.0517 | -0.1187 | 0.1040 |

| | 16: 36.3 | 17: 38.7 | 18: 40.3 | 19: 42.1 | 20: 45.0 | 21: 46.2 | 22: 48.1 | 23: 48.5 | 24: 50.6 |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.1102 | 0.0178 | 0.0948 | 0.3025 | -0.0540 | -0.0132 | 0.1659 | -0.0118 | -0.0071 |
| y | -0.0550 | -0.1327 | 0.0746 | -0.0163 | 0.2252 | 0.0537 | -0.0163 | 0.1431 | 0.0809 |
| z | -0.1268 | -0.0202 | -0.1632 | -0.0809 | -0.1728 | -0.1132 | -0.1256 | 0.0037 | -0.0171 |
| Sn x | 0.0116 | -0.1736 | -0.0015 | -0.0978 | 0.0213 | -0.0802 | -0.0677 | -0.0479 | 0.0022 |
| y | -0.1622 | 0.2075 | 0.0132 | 0.0241 | -0.0494 | 0.0407 | 0.0810 | -0.1311 | 0.0867 |
| z | -0.0170 | -0.0122 | 0.1004 | -0.1376 | -0.0458 | 0.0858 | -0.0361 | -0.0215 | 0.1139 |
| Sn x | -0.0600 | 0.0911 | -0.0875 | 0.0504 | -0.2646 | 0.0601 | 0.0566 | 0.2034 | -0.0207 |
| y | 0.0147 | 0.0060 | 0.0389 | -0.0542 | -0.0528 | 0.0522 | -0.1526 | -0.1377 | 0.1608 |
| z | 0.0258 | -0.0983 | 0.1352 | -0.0266 | -0.2015 | -0.1025 | -0.0302 | -0.0630 | 0.0721 |
| Ag x | 0.1326 | 0.0713 | 0.1623 | -0.1510 | -0.3505 | 0.0351 | -0.0517 | -0.0343 | 0.0018 |
| y | -0.2055 | -0.0412 | 0.1981 | -0.0071 | -0.0560 | 0.0604 | -0.1323 | 0.2671 | -0.0277 |
| z | -0.0413 | -0.0119 | -0.0918 | 0.0687 | -0.1631 | -0.0341 | 0.1744 | -0.0121 | -0.0784 |
| Ag x | -0.0782 | 0.0502 | 0.0298 | 0.1017 | -0.0746 | -0.1153 | -0.1577 | -0.1586 | -0.1127 |
| y | 0.2839 | 0.0373 | 0.0210 | -0.0928 | 0.1019 | 0.1968 | 0.0870 | 0.0362 | -0.0920 |
| z | -0.1210 | -0.0206 | 0.1754 | -0.0562 | 0.1897 | 0.0586 | -0.0505 | -0.0289 | -0.0010 |
| Ag x | 0.0117 | 0.0746 | -0.1289 | -0.3114 | 0.2300 | 0.1878 | 0.2792 | 0.0963 | 0.0233 |
| y | 0.0642 | -0.0913 | 0.0505 | -0.0190 | -0.0396 | -0.1554 | 0.1677 | -0.1751 | 0.1177 |
| z | 0.0618 | 0.0152 | -0.1537 | -0.0782 | 0.1234 | 0.1515 | -0.0910 | 0.0106 | -0.2946 |
| Ag x | 0.0330 | 0.0227 | -0.1081 | -0.0699 | 0.0616 | -0.0616 | -0.1131 | -0.0278 | -0.0458 |
| y | 0.1306 | -0.1499 | -0.0153 | -0.1105 | 0.0599 | -0.2637 | 0.1057 | 0.4229 | -0.0046 |
| z | 0.1215 | -0.0487 | -0.2206 | 0.0516 | -0.0523 | 0.0531 | -0.1154 | -0.0020 | 0.3596 |
| Ag x | -0.1096 | 0.0643 | -0.1651 | -0.0248 | 0.0994 | 0.3141 | 0.0434 | 0.0377 | 0.1281 |
| y | 0.0245 | 0.0217 | -0.1775 | 0.1389 | -0.1281 | -0.1239 | 0.0411 | 0.0027 | -0.0156 |
| z | -0.1530 | 0.0124 | 0.1809 | -0.0807 | 0.0957 | 0.1194 | -0.0587 | 0.0476 | 0.1955 |
| Ag x | 0.0187 | -0.0533 | -0.1036 | -0.0468 | -0.0232 | 0.0751 | -0.0454 | 0.1227 | 0.0051 |
| y | -0.3440 | 0.0948 | -0.1133 | 0.2453 | 0.1263 | -0.1297 | 0.0859 | 0.0813 | -0.0751 |
| z | -0.0016 | -0.1313 | 0.0658 | -0.0681 | -0.0563 | 0.0849 | 0.0297 | 0.1031 | -0.1299 |
| Sn x | -0.2007 | 0.0638 | -0.0309 | 0.0582 | -0.0807 | 0.1756 | -0.0969 | 0.0758 | 0.2054 |
| y | 0.0612 | 0.0038 | 0.0148 | 0.0786 | 0.1128 | 0.0693 | -0.0723 | -0.2969 | 0.1859 |
| z | -0.1253 | 0.0260 | -0.2645 | -0.0322 | -0.1477 | 0.0389 | 0.0491 | 0.1382 | 0.0682 |
| Sn x | 0.0548 | -0.0995 | 0.1404 | 0.2260 | 0.0104 | 0.0374 | 0.1231 | 0.0400 | 0.0636 |
| y | -0.0278 | 0.1307 | -0.0007 | 0.0240 | -0.0886 | 0.0799 | 0.1245 | -0.0928 | -0.1427 |
| z | -0.2556 | -0.0789 | 0.1556 | 0.0819 | 0.1167 | -0.0309 | -0.0756 | 0.0456 | -0.1331 |
| Sn x | 0.1516 | 0.2245 | -0.0365 | -0.0087 | 0.1348 | -0.1560 | -0.1700 | -0.0900 | -0.1116 |
| y | 0.1174 | -0.0871 | 0.0591 | -0.1168 | -0.1276 | 0.0912 | 0.1595 | -0.0340 | 0.1963 |
| z | 0.0120 | -0.1512 | -0.1760 | 0.0077 | 0.0410 | -0.0187 | 0.1545 | -0.0566 | 0.1105 |
| Sn x | 0.1176 | 0.1020 | 0.0198 | 0.1055 | 0.1603 | 0.1347 | 0.0505 | 0.0224 | 0.0014 |
| y | -0.0568 | 0.0297 | 0.1467 | 0.0618 | -0.0460 | -0.0588 | -0.2236 | 0.1383 | 0.0586 |
| z | 0.0190 | -0.0652 | -0.1115 | 0.1904 | -0.1173 | -0.1331 | 0.1255 | -0.0541 | 0.1214 |
| Ag x | 0.1818 | 0.2063 | -0.0312 | -0.0475 | -0.0116 | -0.0408 | -0.0359 | -0.0909 | -0.0171 |
| y | -0.0509 | -0.0021 | -0.0753 | 0.1668 | 0.0381 | -0.0118 | -0.0030 | -0.0212 | -0.0965 |
| z | 0.2614 | -0.1663 | 0.0166 | 0.2082 | -0.2423 | 0.1545 | -0.1120 | -0.0512 | -0.0679 |
| Ag x | 0.0500 | -0.0184 | -0.0808 | 0.1019 | -0.0743 | -0.2788 | -0.1624 | 0.0672 | -0.2023 |
| y | 0.0763 | -0.2360 | -0.0658 | 0.0112 | 0.0926 | 0.0846 | -0.0944 | -0.0011 | -0.2117 |
| z | 0.0504 | 0.1467 | -0.1100 | -0.0185 | 0.0845 | -0.0024 | -0.0784 | 0.0826 | -0.2026 |
| Sn x | 0.1331 | -0.0900 | 0.0992 | 0.2139 | -0.0361 | 0.0442 | 0.1938 | 0.0207 | 0.0994 |
| y | -0.0965 | -0.0716 | -0.0904 | -0.1830 | -0.0308 | -0.0809 | -0.1514 | -0.0942 | 0.0203 |
| z | 0.0049 | 0.2406 | -0.1286 | -0.1101 | -0.0364 | 0.0270 | -0.0030 | 0.0244 | 0.0983 |
| Ag x | 0.0045 | 0.0606 | -0.1241 | -0.0517 | 0.0243 | -0.0179 | -0.1143 | -0.0528 | 0.0310 |
| y | -0.0232 | 0.0100 | -0.0109 | 0.1289 | 0.0426 | 0.1020 | -0.0783 | -0.1712 | -0.0356 |
| z | 0.0480 | -0.1910 | 0.0984 | -0.0325 | -0.0339 | 0.2841 | -0.0684 | 0.0922 | -0.2377 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.0575 | -0.1067 | 0.1011 | -0.1170 | 0.0134 | -0.1863 | 0.0970 | 0.1137 | 0.0484 |
| y | -0.1053 | -0.0305 | 0.1155 | 0.0124 | -0.1485 | 0.2193 | 0.0262 | -0.1113 | -0.1478 |
| z | 0.0996 | -0.0058 | -0.0511 | 0.1763 | 0.3183 | -0.1758 | -0.1678 | 0.1611 | 0.2632 |
| Ag x | -0.1831 | -0.1254 | 0.0072 | -0.0295 | 0.1244 | 0.0399 | -0.1138 | -0.2807 | -0.1192 |
| y | 0.1497 | -0.1202 | -0.0312 | -0.1074 | 0.0345 | -0.1018 | 0.1937 | -0.1021 | -0.0309 |
| z | -0.0892 | 0.1759 | 0.1126 | -0.1757 | 0.1340 | -0.1721 | 0.1607 | -0.2575 | 0.0347 |
| Sn x | 0.0355 | 0.0460 | 0.1524 | 0.1696 | 0.1200 | 0.0988 | -0.0430 | 0.0775 | 0.0841 |
| y | 0.1088 | 0.1173 | -0.2877 | 0.0682 | 0.0266 | 0.0617 | 0.1134 | 0.0713 | -0.1357 |
| z | 0.2281 | -0.0925 | 0.1290 | 0.1761 | 0.2226 | -0.1084 | 0.0893 | -0.1024 | -0.0753 |
| Sn x | -0.1692 | -0.1461 | 0.1042 | -0.1781 | -0.0299 | -0.1529 | 0.3049 | 0.0334 | -0.0815 |
| y | 0.2110 | 0.2942 | 0.2559 | -0.1055 | -0.0608 | -0.1030 | -0.1586 | 0.2335 | 0.0535 |
| z | -0.0658 | 0.1618 | 0.0922 | -0.0361 | -0.0144 | -0.0807 | 0.1587 | -0.0539 | -0.1390 |
| Ag x | 0.0366 | -0.2785 | -0.0402 | -0.2308 | -0.0002 | -0.0978 | -0.1725 | -0.1373 | 0.0105 |
| y | -0.1155 | -0.0132 | -0.1369 | -0.1372 | -0.0206 | -0.1035 | -0.0895 | -0.0125 | 0.0350 |
| z | 0.0740 | 0.3201 | 0.2229 | -0.0374 | -0.0402 | -0.0559 | 0.0642 | -0.0069 | -0.0845 |

25: 51.7 26: 53.2 27: 55.0 28: 57.1 29: 58.2 30: 60.1 31: 63.4 32: 65.6 33: 68.2

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.0704 | 0.1359 | 0.1873 | 0.0109 | -0.1313 | 0.0033 | 0.2012 | -0.0635 | 0.0717 |
| y | 0.1897 | -0.1543 | -0.2021 | -0.0020 | 0.1455 | 0.0604 | -0.1751 | -0.1110 | 0.0827 |
| z | -0.2183 | -0.0495 | -0.2379 | 0.0685 | -0.0204 | -0.0131 | -0.0451 | 0.0051 | -0.1319 |
| Sn x | -0.0759 | 0.0195 | 0.0670 | -0.0206 | -0.0332 | -0.0387 | -0.0210 | -0.0062 | 0.0085 |
| y | 0.1286 | 0.0853 | -0.1610 | -0.1113 | -0.0189 | 0.0018 | -0.1981 | -0.1085 | 0.0551 |
| z | 0.2217 | 0.0323 | -0.0749 | 0.0326 | 0.0531 | 0.0556 | -0.2581 | 0.1566 | -0.0521 |
| Sn x | 0.1125 | -0.1621 | 0.0459 | -0.0018 | -0.1770 | 0.0527 | -0.1962 | 0.1365 | 0.0688 |
| y | -0.1188 | 0.0684 | 0.0326 | -0.0784 | -0.0104 | 0.0022 | -0.0865 | 0.1132 | -0.1058 |
| z | -0.1063 | 0.0739 | -0.1522 | 0.0779 | -0.1430 | 0.0520 | -0.1561 | 0.1148 | 0.0700 |
| Ag x | 0.0528 | 0.0431 | -0.1378 | 0.0404 | -0.0774 | -0.1091 | 0.0345 | -0.0557 | 0.0276 |
| y | -0.0596 | -0.1699 | 0.0524 | 0.2136 | -0.2928 | -0.0051 | 0.0215 | 0.0008 | -0.0868 |
| z | -0.0176 | 0.0710 | 0.2875 | 0.1569 | -0.0675 | 0.0050 | 0.0668 | 0.0104 | -0.0224 |
| Ag x | -0.0612 | -0.1088 | 0.0204 | -0.0333 | -0.0772 | -0.0539 | 0.0922 | 0.1560 | 0.0684 |
| y | -0.0711 | -0.0851 | -0.0551 | 0.1218 | 0.0623 | 0.0225 | 0.0158 | 0.1449 | 0.0974 |
| z | 0.1038 | 0.0559 | 0.0144 | 0.1071 | 0.1251 | -0.0450 | 0.0095 | 0.0681 | 0.2053 |
| Ag x | 0.0667 | 0.1480 | -0.2688 | -0.0111 | -0.2943 | -0.0419 | 0.2836 | 0.1709 | 0.1135 |
| y | -0.0370 | -0.2510 | 0.0222 | 0.0606 | 0.1031 | -0.0314 | -0.0937 | -0.0696 | -0.2491 |
| z | 0.0110 | 0.1279 | 0.0339 | -0.0819 | -0.1336 | 0.3888 | -0.0707 | -0.1448 | -0.1038 |
| Ag x | 0.0799 | 0.0117 | -0.1808 | -0.2043 | 0.0595 | -0.1116 | 0.0589 | 0.0196 | -0.0466 |
| y | -0.0583 | 0.1625 | 0.0962 | -0.1474 | 0.0069 | -0.4234 | -0.2491 | -0.1388 | 0.1883 |
| z | 0.2274 | 0.1959 | 0.0843 | 0.2640 | 0.0364 | 0.0668 | 0.1828 | -0.0018 | 0.1994 |
| Ag x | -0.1779 | 0.0039 | -0.0093 | 0.0271 | 0.1934 | -0.0429 | 0.0098 | -0.0528 | -0.0441 |
| y | 0.0962 | 0.1109 | -0.0887 | 0.0279 | -0.0045 | 0.0325 | 0.0501 | 0.1108 | 0.2559 |
| z | 0.0668 | 0.1211 | 0.1532 | -0.1104 | 0.0650 | -0.0202 | -0.0559 | -0.1433 | -0.1614 |
| Ag x | 0.0813 | -0.1877 | -0.0396 | -0.1496 | 0.0066 | -0.0314 | -0.1231 | -0.0373 | 0.0854 |
| y | 0.0729 | -0.0102 | -0.1559 | 0.0982 | 0.0337 | -0.0214 | 0.1773 | -0.0431 | -0.0792 |
| z | -0.0307 | -0.0952 | 0.2504 | 0.1278 | -0.0151 | -0.0883 | 0.1639 | -0.1536 | 0.0054 |
| Sn x | -0.0760 | 0.0143 | 0.1171 | -0.1780 | -0.0117 | 0.0307 | -0.0454 | -0.0578 | -0.1384 |
| y | -0.1620 | 0.2089 | 0.0018 | -0.2110 | 0.0366 | -0.0509 | 0.0548 | -0.0959 | 0.0017 |
| z | -0.1563 | 0.0402 | -0.1060 | 0.0162 | 0.0288 | 0.0859 | -0.0121 | -0.1816 | -0.1008 |
| Sn x | -0.0210 | 0.1554 | -0.1709 | 0.0778 | -0.0225 | 0.0794 | -0.0790 | 0.0061 | -0.0597 |
| y | -0.0899 | -0.0151 | 0.0371 | -0.0314 | -0.0972 | -0.1024 | 0.1439 | -0.2589 | -0.0124 |
| z | 0.1233 | 0.1966 | -0.1751 | 0.0743 | 0.2088 | -0.1174 | 0.1167 | 0.1178 | -0.1612 |
| Sn x | 0.0374 | 0.1746 | 0.1222 | 0.2872 | 0.0389 | -0.0275 | -0.1826 | -0.1277 | -0.0884 |
| y | 0.0167 | -0.0969 | -0.0395 | 0.0710 | 0.1727 | 0.1404 | 0.1823 | 0.0560 | -0.1808 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| z | 0.0918 | -0.0105 | 0.0353 | 0.1510 | -0.0931 | -0.2982 | -0.1620 | -0.0361 | -0.1334 |
| Sn x | 0.0446 | -0.1346 | 0.1833 | 0.0074 | 0.0567 | -0.0292 | -0.0673 | 0.1172 | -0.1498 |
| y | 0.1771 | 0.0263 | -0.0529 | -0.0335 | -0.2782 | -0.0096 | 0.1097 | -0.2115 | 0.0270 |
| z | 0.0612 | 0.1136 | 0.1034 | -0.3354 | -0.0323 | 0.2333 | -0.1430 | 0.1891 | 0.2171 |
| Ag x | 0.1074 | 0.1726 | 0.0595 | 0.2249 | 0.0253 | -0.0960 | -0.0036 | -0.0998 | -0.0759 |
| y | 0.0140 | -0.0173 | 0.1464 | 0.1347 | 0.2621 | 0.0335 | -0.2039 | 0.0914 | 0.0699 |
| z | 0.1202 | -0.2683 | -0.1061 | -0.2170 | 0.1591 | -0.1235 | 0.2386 | -0.2612 | 0.0480 |
| Ag x | 0.0818 | -0.0194 | -0.1753 | 0.0056 | 0.1635 | 0.0033 | 0.0630 | 0.2038 | -0.2227 |
| y | -0.0881 | 0.2234 | 0.0666 | -0.1153 | -0.1760 | 0.1564 | -0.0624 | -0.0790 | -0.0684 |
| z | -0.1466 | 0.0633 | 0.0152 | -0.1669 | 0.0209 | -0.0257 | -0.0486 | -0.0323 | -0.0417 |
| Sn x | -0.1837 | 0.0703 | -0.2147 | 0.1669 | -0.0638 | 0.0691 | -0.1169 | -0.1170 | -0.0806 |
| y | 0.1954 | -0.0067 | 0.1241 | 0.0004 | 0.0060 | 0.1159 | 0.1557 | 0.0864 | -0.0531 |
| z | -0.1542 | -0.1402 | 0.0123 | 0.0759 | 0.1401 | -0.1298 | 0.0398 | -0.0624 | 0.1482 |
| Ag x | 0.0724 | -0.0421 | -0.1275 | -0.1759 | 0.0513 | -0.1356 | 0.0273 | -0.0107 | -0.0091 |
| y | -0.2961 | 0.0412 | 0.0118 | -0.0707 | -0.0763 | -0.1853 | 0.0501 | 0.1326 | 0.0697 |
| z | 0.0574 | 0.0004 | -0.0345 | -0.0280 | 0.0286 | -0.0352 | 0.0055 | 0.1945 | 0.0017 |
| Sn x | -0.1519 | -0.0121 | 0.0446 | -0.0150 | 0.1362 | 0.1575 | 0.1281 | -0.0186 | 0.0936 |
| y | -0.1416 | 0.0811 | 0.0085 | 0.0856 | 0.0606 | -0.1909 | -0.0567 | 0.3173 | 0.1187 |
| z | -0.3348 | -0.2466 | -0.0288 | 0.0511 | -0.1627 | 0.1001 | 0.1153 | 0.1794 | -0.0005 |
| Ag x | -0.0275 | -0.2560 | -0.0896 | 0.2013 | -0.0215 | 0.1952 | -0.1847 | -0.2835 | 0.4170 |
| y | 0.1025 | -0.0572 | -0.0650 | 0.0024 | -0.1816 | 0.1667 | -0.0365 | -0.0077 | -0.2618 |
| z | 0.0999 | -0.2349 | 0.0637 | -0.1162 | -0.2459 | -0.1163 | 0.0067 | 0.0829 | 0.0516 |
| Sn x | 0.1764 | -0.1205 | 0.2298 | -0.1678 | -0.0567 | -0.0099 | -0.0284 | 0.1094 | -0.0992 |
| y | 0.0910 | -0.1864 | 0.1173 | 0.0189 | 0.0445 | 0.0472 | -0.0220 | 0.0929 | 0.0151 |
| z | 0.0827 | -0.0024 | -0.0896 | -0.0178 | -0.0142 | -0.0712 | 0.1281 | -0.0845 | 0.0631 |
| Sn x | -0.1202 | 0.0501 | 0.1073 | -0.1328 | 0.2864 | 0.1778 | 0.1247 | -0.0386 | 0.0779 |
| y | -0.0875 | 0.0627 | 0.0172 | -0.0094 | 0.1322 | 0.2040 | 0.0857 | -0.0163 | 0.1440 |
| z | -0.0231 | -0.0237 | -0.0086 | -0.1021 | 0.0079 | -0.0447 | -0.0949 | -0.0453 | -0.0756 |
| Ag x | -0.0790 | 0.0345 | 0.1951 | 0.0390 | -0.0523 | -0.0641 | 0.0387 | 0.0528 | -0.0033 |
| y | 0.1163 | -0.0242 | 0.0918 | -0.0100 | 0.0601 | 0.0261 | 0.1276 | 0.0005 | -0.0327 |
| z | -0.0591 | -0.0200 | -0.0049 | -0.0319 | 0.0553 | 0.1483 | -0.0041 | 0.0107 | -0.0172 |

34: 70.2 35: 72.5 36: 73.9 37: 75.2 38: 79.5 39: 82.6 40: 83.6 41: 86.5 42: 89.9

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.1088 | -0.1219 | 0.1906 | -0.1941 | 0.1871 | 0.2089 | 0.1325 | 0.4374 | -0.1171 |
| y | 0.0147 | 0.2271 | 0.2136 | 0.0746 | -0.1631 | 0.1954 | 0.0250 | 0.2358 | 0.1590 |
| z | -0.1802 | 0.2527 | -0.2527 | 0.0618 | 0.2743 | 0.1250 | 0.1275 | -0.1076 | 0.0229 |
| Sn x | -0.0161 | 0.0059 | 0.0436 | 0.0403 | 0.0618 | -0.1104 | -0.0052 | 0.0021 | -0.1332 |
| y | -0.0889 | -0.0954 | 0.0926 | 0.2697 | 0.0927 | 0.1058 | 0.1033 | -0.2278 | -0.0084 |
| z | 0.0113 | -0.0764 | -0.0380 | -0.1453 | -0.0188 | 0.2605 | -0.1566 | -0.0008 | 0.0047 |
| Sn x | -0.0508 | -0.1453 | 0.1804 | -0.0769 | 0.0061 | -0.2668 | -0.0916 | -0.1969 | 0.1275 |
| y | -0.0513 | -0.0885 | -0.2890 | 0.1178 | 0.1412 | 0.1011 | 0.2125 | 0.2126 | -0.2826 |
| z | -0.1483 | -0.2310 | 0.1108 | -0.0582 | -0.0395 | -0.1207 | 0.1069 | 0.1966 | 0.1439 |
| Ag x | 0.0367 | -0.0447 | 0.1036 | 0.0637 | -0.0350 | -0.0525 | -0.1566 | 0.1367 | -0.1186 |
| y | -0.1072 | -0.2891 | -0.0133 | -0.0663 | -0.0529 | -0.0351 | 0.0661 | -0.0927 | 0.0593 |
| z | 0.0771 | -0.1166 | -0.0407 | 0.0046 | -0.0381 | 0.1913 | -0.1858 | -0.3383 | -0.0764 |
| Ag x | -0.0834 | 0.2166 | -0.0155 | 0.0217 | 0.1162 | 0.0955 | 0.0052 | -0.0367 | 0.3355 |
| y | -0.0076 | -0.0537 | -0.1078 | 0.0219 | 0.0760 | 0.0006 | -0.2703 | 0.0449 | -0.0489 |
| z | 0.0044 | -0.1747 | -0.0085 | 0.1346 | 0.1897 | -0.0144 | -0.0417 | 0.0183 | 0.0023 |
| Ag x | 0.0989 | -0.0531 | 0.0123 | 0.0419 | -0.0026 | 0.0327 | 0.3503 | -0.0864 | 0.1010 |
| y | 0.1192 | -0.1140 | 0.0103 | -0.1193 | 0.0280 | -0.0045 | -0.0338 | 0.0666 | 0.0598 |
| z | -0.0517 | -0.0252 | 0.0867 | 0.0667 | 0.2225 | -0.0812 | 0.0011 | 0.0582 | -0.1501 |
| Ag x | -0.0189 | -0.2561 | -0.2551 | -0.3359 | -0.1559 | 0.0571 | -0.0901 | 0.0719 | 0.1088 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| y | -0.0590 | 0.0110 | -0.0883 | -0.0053 | 0.0182 | 0.0155 | -0.0348 | -0.0201 | -0.0501 |
| z | -0.2127 | 0.1199 | -0.1277 | -0.0233 | -0.2026 | -0.0337 | 0.0479 | -0.0842 | -0.0582 |
| Ag x | -0.1382 | -0.1237 | 0.1158 | 0.0755 | -0.1102 | -0.0030 | -0.1603 | 0.0721 | -0.0513 |
| y | 0.0570 | -0.0921 | 0.0056 | 0.1712 | 0.1020 | -0.0151 | -0.2189 | 0.0533 | -0.0841 |
| z | 0.0575 | -0.0001 | 0.1257 | -0.0621 | -0.1596 | -0.0458 | 0.3163 | -0.1356 | 0.0442 |
| Ag x | -0.1126 | 0.2034 | 0.1875 | -0.0134 | 0.3267 | -0.0804 | 0.0760 | -0.1813 | -0.1633 |
| y | -0.0561 | -0.0010 | -0.1175 | -0.2828 | 0.1018 | 0.0940 | -0.0679 | -0.0852 | -0.1006 |
| z | 0.0418 | 0.1332 | 0.0775 | 0.1509 | -0.0012 | 0.0024 | 0.0033 | 0.0341 | -0.0447 |
| Sn x | 0.0615 | 0.1233 | -0.0083 | -0.0070 | -0.1213 | 0.0183 | -0.1860 | 0.0391 | 0.0163 |
| y | -0.0521 | 0.0277 | 0.2628 | -0.2319 | 0.0732 | -0.2318 | -0.1998 | -0.2843 | 0.0434 |
| z | -0.0197 | 0.0978 | 0.1008 | -0.0192 | -0.1404 | 0.1216 | -0.1468 | 0.2200 | -0.1132 |
| Sn x | -0.0850 | 0.0158 | -0.0354 | 0.1111 | -0.0605 | 0.0440 | -0.0622 | 0.0132 | 0.0305 |
| y | -0.0203 | 0.1129 | -0.1603 | 0.0460 | -0.1249 | -0.4352 | 0.1276 | 0.2099 | 0.0996 |
| z | 0.0985 | -0.0558 | -0.1223 | 0.2808 | -0.0404 | -0.3630 | -0.1612 | 0.0047 | 0.0119 |
| Sn x | -0.0133 | 0.1091 | -0.0201 | -0.1713 | -0.0253 | -0.0176 | 0.1258 | 0.0163 | 0.0887 |
| y | 0.1637 | 0.0309 | 0.0606 | -0.0118 | 0.3088 | -0.0177 | -0.0235 | 0.0431 | 0.2659 |
| z | 0.1107 | 0.0404 | 0.0602 | -0.0360 | 0.2377 | -0.0814 | 0.0290 | 0.1251 | 0.0902 |
| Sn x | -0.1026 | -0.0338 | -0.0840 | 0.0701 | 0.0161 | -0.0322 | -0.0109 | 0.0216 | -0.0115 |
| y | 0.3468 | 0.1360 | -0.0448 | -0.0106 | 0.0251 | 0.0932 | -0.0922 | -0.0479 | 0.0679 |
| z | 0.2773 | 0.0955 | -0.1249 | -0.0228 | -0.0672 | -0.1583 | 0.1115 | 0.1073 | 0.0869 |
| Ag x | 0.1107 | 0.1296 | 0.0317 | 0.0479 | 0.0983 | 0.0714 | -0.0235 | -0.0127 | 0.0851 |
| y | -0.2028 | -0.1424 | 0.0012 | -0.0230 | 0.0045 | -0.0980 | 0.2859 | -0.0436 | 0.0822 |
| z | -0.1481 | -0.1656 | -0.0480 | 0.1001 | -0.0612 | 0.1310 | 0.1904 | -0.1260 | 0.0162 |
| Ag x | 0.1259 | 0.0414 | 0.2806 | 0.1007 | -0.2383 | 0.0049 | 0.1512 | -0.0532 | -0.1502 |
| y | -0.0956 | -0.0565 | -0.0886 | 0.0032 | -0.0549 | 0.1655 | -0.0898 | -0.0586 | 0.2432 |
| z | 0.0658 | -0.1547 | 0.0983 | 0.0742 | -0.0195 | 0.1249 | -0.0276 | 0.0579 | 0.1335 |
| Sn x | -0.0447 | 0.1051 | -0.2029 | 0.1114 | -0.1107 | -0.0340 | 0.0035 | -0.1402 | 0.0858 |
| y | -0.0854 | -0.0096 | 0.0561 | 0.0227 | -0.0009 | 0.0543 | -0.0205 | -0.0143 | 0.1243 |
| z | 0.2816 | -0.1397 | -0.0936 | -0.1483 | -0.0502 | 0.0211 | 0.1107 | -0.0851 | -0.0228 |
| Ag x | -0.0083 | -0.1140 | -0.0570 | -0.0683 | 0.1034 | -0.0627 | -0.0315 | 0.0629 | -0.0794 |
| y | 0.1158 | 0.0085 | 0.0520 | 0.1075 | -0.1037 | 0.1421 | 0.0484 | -0.0121 | -0.0028 |
| z | -0.0293 | 0.2500 | -0.1123 | -0.4030 | 0.0063 | -0.1314 | -0.0340 | 0.0507 | 0.0088 |
| Sn x | -0.0629 | 0.0134 | -0.0230 | -0.0274 | -0.0205 | -0.0279 | 0.0020 | -0.0142 | 0.0028 |
| y | 0.0953 | 0.2422 | 0.1606 | -0.1132 | -0.1189 | 0.1193 | 0.0971 | -0.0498 | -0.2288 |
| z | 0.0670 | 0.0007 | 0.1302 | 0.0166 | 0.0422 | -0.0686 | -0.0143 | 0.0150 | -0.0489 |
| Ag x | 0.2295 | -0.0355 | -0.1087 | -0.0533 | -0.0589 | -0.0495 | -0.0113 | -0.0050 | -0.1212 |
| y | 0.0571 | -0.0247 | -0.0194 | -0.0951 | -0.1974 | -0.0553 | 0.0861 | -0.1203 | -0.3930 |
| z | -0.4018 | 0.1988 | -0.0338 | 0.0858 | -0.2249 | 0.0275 | -0.1872 | 0.0465 | -0.0033 |
| Sn x | 0.1352 | 0.0384 | -0.2935 | 0.1345 | 0.0839 | 0.0413 | -0.0082 | -0.0413 | -0.1466 |
| y | 0.0414 | 0.0510 | -0.0124 | 0.1202 | -0.1763 | 0.0245 | 0.0143 | 0.0836 | 0.1690 |
| z | -0.0629 | -0.0185 | 0.1727 | -0.0765 | 0.0355 | 0.0402 | -0.0538 | -0.0776 | -0.0736 |
| Sn x | -0.0207 | 0.0477 | -0.0799 | -0.0272 | 0.0236 | 0.0942 | 0.0216 | -0.1149 | 0.0418 |
| y | -0.1275 | 0.0695 | -0.0137 | -0.0441 | 0.0026 | -0.0552 | 0.0104 | 0.0144 | -0.1005 |
| z | 0.0645 | -0.0161 | 0.0233 | 0.0592 | 0.0409 | -0.0195 | -0.0392 | 0.0361 | -0.0600 |
| Ag x | 0.0828 | -0.1292 | 0.0537 | 0.1577 | -0.0859 | 0.0727 | -0.0269 | 0.0084 | 0.0694 |
| y | -0.0688 | 0.0158 | 0.0238 | 0.0370 | 0.0162 | -0.1611 | -0.0378 | 0.0838 | -0.0890 |
| z | 0.0728 | -0.0123 | 0.0180 | -0.0364 | 0.0010 | 0.0844 | 0.0080 | -0.0364 | 0.0835 |

43: 91.6 44: 92.7 45: 96.3 46: 100.0 47: 102.7 48: 106.4 49: 107.9 50: 109.9 51: 113.7

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.0569 | 0.1996 | -0.0158 | -0.0804 | 0.0272 | -0.1055 | 0.0497 | -0.0470 | -0.1059 |
| y | -0.0201 | 0.0386 | 0.0190 | -0.0722 | 0.0605 | -0.0103 | 0.0132 | 0.0525 | -0.1321 |
| z | -0.0729 | 0.1686 | -0.0228 | -0.1736 | -0.0882 | -0.0093 | 0.0942 | -0.0522 | -0.2880 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.0668 | -0.2067 | 0.3404 | -0.0883 | -0.0679 | -0.1752 | -0.0686 | 0.2825 | 0.3366 |
| y | 0.1656 | 0.0890 | 0.0706 | 0.1898 | 0.0707 | 0.0491 | -0.1446 | 0.1645 | -0.0866 |
| z | -0.0689 | -0.1215 | -0.0734 | -0.2796 | -0.1036 | -0.0156 | 0.1437 | -0.1393 | 0.1485 |
| Sn x | 0.0171 | 0.0684 | 0.0215 | -0.0559 | 0.0552 | -0.1083 | 0.1012 | -0.1269 | -0.1329 |
| y | 0.0016 | 0.0108 | 0.1398 | 0.1808 | 0.1016 | -0.0180 | -0.0667 | -0.0771 | 0.1060 |
| z | 0.0067 | -0.0380 | -0.0164 | -0.0332 | 0.2113 | -0.2273 | 0.0847 | 0.0110 | 0.0314 |
| Ag x | -0.2832 | 0.0915 | -0.0136 | -0.0944 | -0.1657 | 0.1403 | -0.2832 | -0.0623 | 0.0760 |
| y | 0.2468 | -0.0711 | -0.0455 | 0.0791 | -0.1186 | 0.2377 | 0.1566 | 0.1939 | 0.1215 |
| z | -0.0657 | -0.2236 | 0.1091 | 0.1657 | 0.1581 | -0.0412 | -0.2085 | -0.0353 | -0.1317 |
| Ag x | -0.0528 | -0.0058 | -0.0490 | -0.2506 | 0.2080 | -0.0032 | -0.1970 | 0.2883 | 0.1166 |
| y | 0.2137 | 0.0226 | -0.1114 | 0.0146 | -0.0353 | -0.1277 | -0.1114 | -0.0760 | 0.0620 |
| z | -0.0657 | 0.0624 | 0.1331 | 0.0119 | -0.0625 | 0.1221 | 0.2309 | 0.1012 | -0.1483 |
| Ag x | 0.0802 | -0.0514 | 0.0024 | -0.0694 | -0.1011 | -0.0786 | -0.1287 | -0.0538 | -0.0303 |
| y | 0.1255 | 0.1220 | 0.1256 | -0.0555 | -0.0783 | 0.0075 | -0.1564 | 0.1438 | -0.2075 |
| z | -0.1291 | -0.1542 | -0.3664 | 0.0585 | 0.0771 | 0.0179 | -0.0139 | 0.2458 | -0.0776 |
| Ag x | -0.1794 | -0.0253 | 0.0562 | 0.1719 | -0.1241 | -0.0655 | -0.0771 | 0.2751 | -0.2162 |
| y | -0.0775 | 0.0571 | -0.2119 | 0.1083 | 0.0676 | -0.1174 | 0.0960 | 0.1036 | 0.0765 |
| z | 0.0722 | 0.0556 | 0.0753 | -0.0353 | -0.0243 | -0.1194 | 0.0368 | 0.0541 | -0.0596 |
| Ag x | -0.0407 | 0.0040 | 0.0678 | 0.0245 | 0.0166 | 0.2047 | 0.0403 | 0.0858 | -0.0449 |
| y | -0.2137 | 0.0681 | 0.1814 | -0.0540 | 0.1698 | 0.2312 | 0.1884 | 0.1204 | -0.0168 |
| z | -0.3092 | -0.0894 | 0.0715 | -0.0649 | 0.1530 | 0.1067 | 0.0058 | 0.0175 | 0.0585 |
| Ag x | 0.0613 | 0.1751 | 0.1607 | 0.1012 | -0.0133 | -0.0123 | -0.0358 | -0.0671 | 0.1069 |
| y | -0.0813 | -0.0581 | -0.1209 | -0.0794 | -0.1459 | 0.1013 | 0.0430 | -0.0963 | 0.1784 |
| z | -0.0412 | 0.1572 | -0.0547 | -0.1607 | -0.2544 | 0.0154 | -0.0163 | 0.0270 | 0.1221 |
| Sn x | 0.0549 | 0.0116 | -0.0855 | -0.0718 | 0.1004 | -0.0992 | -0.1161 | 0.0860 | 0.0483 |
| y | 0.0535 | 0.1116 | -0.1088 | -0.0861 | -0.1397 | -0.0421 | 0.0929 | -0.0829 | -0.0977 |
| z | 0.1580 | -0.0170 | -0.0015 | 0.1684 | 0.0127 | -0.0971 | -0.0458 | -0.0635 | 0.1058 |
| Sn x | 0.0804 | 0.0290 | -0.0838 | 0.1089 | 0.0323 | -0.0446 | -0.1122 | -0.0556 | -0.0569 |
| y | -0.1704 | 0.0082 | 0.0870 | 0.1067 | 0.0334 | 0.0250 | 0.1308 | -0.1079 | -0.0883 |
| z | 0.1722 | 0.1858 | -0.1077 | -0.0855 | 0.0683 | -0.1667 | -0.1519 | 0.0244 | 0.0690 |
| Sn x | 0.3175 | 0.0239 | -0.0220 | 0.0560 | -0.0045 | 0.0923 | 0.0086 | 0.1471 | -0.0101 |
| y | -0.0640 | -0.1375 | 0.0070 | 0.1940 | -0.0046 | -0.0937 | 0.1577 | 0.0127 | 0.1382 |
| z | 0.0873 | -0.1829 | -0.0438 | -0.0285 | 0.0205 | 0.3655 | -0.2086 | -0.1215 | -0.0576 |
| Sn x | -0.0117 | 0.0651 | -0.0346 | -0.0383 | -0.0651 | -0.0522 | 0.1946 | -0.0294 | -0.0172 |
| y | 0.0185 | -0.1023 | 0.0125 | 0.0814 | 0.0199 | -0.2285 | -0.0677 | -0.1420 | -0.1188 |
| z | 0.1937 | -0.0021 | -0.1078 | 0.0388 | -0.3145 | 0.2094 | 0.0265 | 0.0767 | 0.1109 |
| Ag x | -0.0455 | -0.0317 | 0.0131 | 0.0812 | -0.0201 | -0.1507 | 0.2821 | -0.0120 | 0.1178 |
| y | -0.2070 | -0.0804 | -0.0805 | 0.0011 | -0.1156 | -0.2444 | -0.3062 | -0.2832 | 0.0721 |
| z | 0.1739 | -0.1010 | -0.1410 | -0.0049 | -0.0724 | -0.0375 | 0.0839 | 0.0684 | 0.0065 |
| Ag x | 0.0199 | -0.0405 | 0.1092 | 0.1603 | -0.0296 | 0.1204 | 0.1673 | -0.1695 | 0.0138 |
| y | -0.0804 | 0.1697 | 0.3101 | -0.1303 | -0.1323 | 0.0454 | 0.0350 | -0.1287 | 0.1754 |
| z | 0.1043 | 0.0393 | 0.2543 | -0.0076 | -0.1960 | -0.0209 | -0.0738 | -0.1862 | -0.0630 |
| Sn x | -0.1667 | -0.1193 | -0.0145 | 0.0349 | -0.0793 | 0.1343 | 0.0866 | 0.0161 | 0.0576 |
| y | -0.0595 | 0.2278 | -0.1592 | 0.2792 | 0.0474 | 0.0973 | -0.0626 | -0.0605 | 0.1421 |
| z | 0.0057 | 0.3047 | 0.0090 | -0.0954 | 0.1657 | 0.0079 | 0.0030 | 0.0175 | 0.1482 |
| Ag x | -0.0373 | -0.2200 | -0.2249 | -0.0625 | 0.1152 | 0.0687 | 0.0620 | -0.1574 | 0.1783 |
| y | 0.1784 | -0.1214 | -0.0671 | -0.1361 | 0.2502 | 0.0823 | 0.1187 | -0.1415 | 0.0945 |
| z | 0.0806 | 0.0379 | 0.1967 | 0.1831 | 0.2860 | 0.1150 | -0.0069 | -0.0760 | -0.0853 |
| Sn x | -0.0178 | 0.0591 | -0.0329 | 0.0122 | -0.0643 | 0.1620 | -0.1877 | -0.0137 | 0.0218 |
| y | -0.1160 | -0.0693 | -0.1226 | 0.1192 | -0.2707 | -0.0818 | 0.0072 | 0.2473 | -0.1265 |
| z | -0.1866 | -0.0097 | 0.0033 | 0.1275 | -0.0268 | -0.1382 | -0.0002 | 0.0394 | -0.0581 |
| Ag x | -0.0111 | -0.0444 | 0.0050 | 0.0574 | -0.0090 | -0.0433 | 0.0110 | -0.1267 | 0.0279 |
| y | 0.0067 | 0.2466 | -0.0539 | -0.2708 | 0.1653 | -0.0393 | 0.0553 | 0.0651 | 0.0134 |
| z | 0.0308 | -0.0558 | -0.0115 | 0.1686 | -0.0555 | 0.0220 | 0.0580 | -0.1322 | 0.0804 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.0416 | 0.0446 | 0.0451 | -0.0039 | -0.0118 | 0.0166 | -0.0217 | -0.0600 | -0.1237 |
| y | -0.0959 | -0.0410 | -0.0396 | -0.1465 | 0.1388 | 0.0003 | -0.0486 | 0.1367 | -0.0131 |
| z | -0.0767 | -0.0426 | 0.0864 | 0.0249 | 0.1379 | 0.0767 | -0.1596 | 0.0336 | 0.0621 |
| Sn x | 0.1232 | -0.0874 | 0.0042 | -0.0140 | 0.1822 | -0.0638 | 0.1676 | -0.0571 | -0.0582 |
| y | 0.1158 | -0.2151 | 0.0176 | -0.2263 | 0.0357 | 0.2330 | -0.1375 | -0.1215 | -0.1858 |
| z | 0.0091 | -0.1768 | 0.0997 | -0.1296 | -0.0731 | -0.1874 | 0.1274 | 0.0368 | -0.1468 |
| Ag x | -0.0137 | 0.0562 | -0.2552 | 0.0278 | 0.0136 | 0.0751 | 0.0519 | -0.1495 | -0.3032 |
| y | 0.0681 | -0.2717 | 0.1547 | -0.1276 | -0.1243 | -0.1034 | 0.0133 | 0.0763 | -0.0840 |
| z | -0.0897 | 0.1999 | -0.0829 | 0.1743 | -0.0199 | 0.0110 | -0.0050 | 0.0594 | 0.1665 |

52: 115.4 53: 115.7 54: 118.9 55: 120.1 56: 121.7 57: 126.1 58: 129.8 59: 133.4 60: 135.6

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.1190 | -0.0048 | 0.0143 | 0.1226 | 0.0382 | 0.0390 | 0.0797 | -0.1041 | -0.1018 |
| y | 0.2715 | -0.0422 | -0.0055 | -0.0485 | 0.0086 | 0.0514 | 0.0541 | -0.0489 | 0.0161 |
| z | 0.2349 | 0.1048 | 0.0522 | 0.2510 | 0.0900 | -0.1108 | 0.0416 | -0.0909 | -0.1079 |
| Sn x | 0.2176 | -0.0107 | 0.2742 | 0.1871 | 0.0054 | -0.1223 | -0.1154 | -0.0180 | 0.0282 |
| y | -0.1329 | -0.2289 | -0.0950 | 0.1570 | -0.1873 | -0.0851 | 0.0572 | -0.0395 | -0.0288 |
| z | 0.0687 | 0.1858 | 0.0644 | -0.1158 | 0.0552 | -0.0000 | -0.0029 | -0.0143 | 0.0744 |
| Sn x | 0.0152 | 0.0901 | 0.0889 | -0.1986 | 0.1212 | 0.0227 | -0.0736 | -0.3396 | 0.2253 |
| y | -0.1142 | 0.0658 | -0.0685 | -0.2194 | 0.0791 | 0.1029 | -0.0466 | -0.1464 | 0.1535 |
| z | -0.3752 | -0.0564 | 0.2245 | 0.1022 | -0.0284 | -0.0748 | 0.0164 | 0.1511 | -0.1160 |
| Ag x | 0.1825 | 0.0281 | -0.2127 | 0.0673 | -0.2731 | -0.0636 | -0.0853 | -0.0005 | -0.1120 |
| y | 0.2169 | -0.0215 | -0.2566 | 0.0529 | 0.0704 | 0.0377 | 0.0107 | 0.0768 | -0.0854 |
| z | 0.2267 | 0.0301 | 0.0547 | 0.0034 | -0.0104 | 0.0876 | 0.1183 | 0.1247 | -0.0846 |
| Ag x | 0.0075 | -0.0121 | -0.1481 | -0.1654 | -0.0434 | 0.2258 | 0.0450 | 0.0844 | 0.2086 |
| y | -0.0402 | 0.0366 | -0.0659 | 0.1348 | 0.1190 | -0.0146 | 0.0040 | -0.0878 | 0.0046 |
| z | 0.0977 | -0.1370 | 0.2338 | -0.3016 | -0.2726 | 0.0018 | -0.0026 | 0.1438 | -0.1064 |
| Ag x | 0.0364 | 0.0509 | 0.0070 | -0.1298 | -0.0210 | -0.1024 | -0.0446 | 0.0641 | 0.0245 |
| y | -0.0402 | 0.3070 | 0.0397 | -0.1382 | -0.1176 | -0.0864 | -0.1291 | 0.2864 | 0.1850 |
| z | 0.0557 | 0.0649 | 0.0850 | -0.0330 | -0.1025 | -0.0165 | -0.0860 | -0.0336 | 0.1291 |
| Ag x | -0.0260 | -0.2216 | 0.0023 | 0.0927 | 0.0424 | -0.0112 | -0.0842 | -0.2190 | 0.1607 |
| y | 0.0512 | 0.1068 | -0.0321 | 0.0009 | -0.0659 | -0.0629 | 0.0359 | -0.0057 | 0.0058 |
| z | -0.0087 | 0.1250 | -0.0887 | -0.0418 | -0.0707 | -0.0457 | -0.0204 | 0.0515 | 0.0145 |
| Ag x | -0.1213 | 0.3506 | 0.1293 | 0.2869 | -0.1547 | 0.3842 | 0.0660 | -0.1168 | 0.0083 |
| y | -0.0522 | 0.0079 | -0.1076 | 0.0097 | 0.2112 | -0.1887 | -0.0336 | 0.0451 | 0.0768 |
| z | -0.0717 | 0.0959 | -0.1875 | 0.1556 | 0.2293 | -0.0918 | -0.0147 | -0.0031 | 0.1302 |
| Ag x | -0.1787 | 0.0939 | -0.0905 | -0.0948 | 0.0303 | 0.1596 | 0.0346 | 0.1472 | -0.0398 |
| y | -0.3010 | 0.0292 | -0.0471 | -0.0291 | -0.1009 | -0.0798 | -0.0715 | 0.0406 | 0.0589 |
| z | -0.3032 | -0.0770 | 0.0265 | 0.0680 | -0.1299 | -0.2012 | -0.1611 | -0.1540 | 0.1575 |
| Sn x | -0.0723 | -0.1567 | -0.0010 | -0.1429 | 0.0579 | -0.2251 | -0.0356 | 0.0602 | -0.3390 |
| y | 0.1275 | -0.1069 | 0.0419 | -0.0046 | 0.0047 | -0.1320 | -0.0106 | 0.0020 | 0.0008 |
| z | 0.1131 | -0.2314 | -0.0773 | -0.3262 | -0.0185 | -0.0056 | -0.0244 | 0.0364 | 0.2000 |
| Sn x | 0.0397 | 0.1002 | -0.0675 | 0.1445 | 0.1775 | -0.0883 | -0.1181 | 0.1547 | 0.0791 |
| y | 0.1507 | 0.1147 | 0.0771 | -0.1650 | 0.1004 | 0.0648 | -0.0071 | 0.0933 | -0.0170 |
| z | 0.0239 | 0.0139 | -0.0335 | 0.0029 | 0.1478 | 0.1546 | 0.0425 | -0.0752 | -0.0109 |
| Sn x | -0.0471 | 0.1970 | 0.0089 | -0.1431 | -0.0362 | -0.0816 | -0.0454 | -0.1800 | -0.2291 |
| y | 0.0175 | -0.0334 | -0.1370 | 0.0273 | -0.0180 | -0.0311 | 0.0438 | -0.2325 | -0.1908 |
| z | -0.0406 | -0.2834 | 0.2037 | 0.0647 | 0.1926 | 0.0679 | 0.0133 | -0.0938 | 0.0302 |
| Sn x | 0.0543 | -0.2359 | 0.0202 | 0.0977 | -0.0670 | -0.0111 | 0.0678 | 0.3023 | 0.2763 |
| y | -0.1327 | 0.1189 | 0.2630 | 0.1508 | -0.1857 | 0.2184 | 0.0597 | 0.0344 | 0.0865 |
| z | 0.0680 | 0.0677 | -0.1152 | 0.1416 | -0.1063 | 0.1774 | 0.0059 | 0.0180 | 0.0206 |
| Ag x | 0.0099 | -0.1831 | -0.1396 | 0.1635 | 0.1289 | 0.1582 | 0.0362 | 0.1506 | 0.1910 |
| y | 0.1411 | -0.0937 | -0.0640 | 0.0271 | -0.2043 | 0.0348 | -0.0018 | -0.0419 | -0.0148 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| z | -0.0072 | -0.0218 | 0.0846 | -0.0416 | 0.1049 | 0.0360 | 0.0286 | 0.0107 | -0.0123 |
| Ag x | 0.0291 | -0.0483 | 0.1111 | 0.0131 | -0.1113 | -0.0472 | -0.0429 | -0.0852 | -0.0477 |
| y | -0.0566 | -0.1251 | 0.0352 | -0.0915 | 0.0194 | 0.2275 | 0.0283 | -0.0688 | -0.1766 |
| z | -0.0731 | 0.1338 | -0.0779 | 0.0375 | 0.2062 | -0.1447 | 0.0551 | 0.2236 | -0.0085 |
| Sn x | -0.1163 | -0.0398 | 0.0832 | -0.1646 | -0.1408 | -0.0074 | 0.0125 | -0.0249 | -0.0176 |
| y | 0.0879 | 0.0854 | 0.2008 | 0.0625 | 0.1007 | -0.0404 | -0.3646 | 0.1591 | 0.0170 |
| z | 0.0637 | -0.1488 | 0.0661 | -0.0003 | -0.0411 | 0.1750 | -0.0866 | -0.0666 | -0.0745 |
| Ag x | 0.0501 | 0.0998 | 0.0149 | -0.0459 | -0.0065 | 0.0393 | 0.1184 | 0.2724 | -0.2470 |
| y | 0.1404 | 0.0958 | 0.0366 | 0.0428 | -0.2112 | -0.2216 | -0.0128 | -0.1536 | 0.2431 |
| z | -0.0308 | -0.0517 | -0.1503 | 0.1378 | -0.2592 | -0.1421 | 0.0724 | 0.1045 | 0.0250 |
| Sn x | -0.0103 | -0.0498 | 0.1514 | -0.0194 | 0.0902 | -0.0710 | 0.3308 | 0.0868 | 0.1052 |
| y | -0.0999 | -0.0084 | 0.1242 | -0.1080 | 0.2743 | 0.1434 | 0.0070 | 0.0785 | -0.1040 |
| z | 0.0036 | -0.0308 | -0.0985 | 0.0285 | -0.0189 | 0.0637 | -0.0711 | 0.0095 | -0.0872 |
| Ag x | -0.0115 | -0.0199 | -0.0884 | 0.0990 | 0.1630 | -0.1138 | 0.0088 | -0.0095 | 0.0012 |
| y | 0.0309 | -0.1392 | -0.0024 | 0.0589 | -0.0142 | 0.1541 | 0.1537 | 0.0288 | -0.0487 |
| z | -0.0206 | -0.0307 | 0.0407 | 0.0792 | -0.0025 | 0.0535 | -0.0142 | -0.1158 | -0.0566 |
| Sn x | 0.0291 | 0.0093 | 0.0881 | -0.0746 | 0.0385 | -0.1729 | -0.0481 | -0.1324 | -0.1162 |
| y | -0.1372 | 0.0074 | 0.0542 | 0.0971 | 0.0269 | -0.1317 | -0.0080 | 0.0524 | -0.2526 |
| z | 0.0013 | 0.1378 | -0.1399 | -0.1669 | 0.1109 | 0.0400 | -0.0427 | -0.1719 | -0.0549 |
| Sn x | -0.0282 | 0.0028 | -0.0177 | 0.0151 | -0.0021 | 0.0642 | -0.2218 | -0.0554 | -0.0309 |
| y | -0.0579 | -0.1996 | 0.0829 | 0.0250 | 0.1049 | 0.1316 | -0.1811 | 0.0343 | 0.0312 |
| z | -0.0397 | 0.0090 | -0.2854 | 0.0036 | -0.1063 | 0.1062 | -0.2655 | 0.0398 | -0.1140 |
| Ag x | -0.1884 | -0.0355 | -0.2600 | -0.1018 | -0.0513 | 0.0567 | 0.1234 | -0.0252 | -0.0213 |
| y | -0.0697 | 0.0346 | -0.1003 | -0.0413 | -0.0296 | -0.1066 | 0.4319 | -0.1059 | 0.0535 |
| z | 0.0077 | 0.1118 | 0.1250 | -0.0480 | 0.0171 | -0.1595 | 0.4164 | -0.0817 | 0.0639 |

61: 144.2 62: 144.6 63: 147.0 64: 149.9 65: 154.2 66: 160.6

| | | | | | | |
|---|---|---|---|---|---|---|
| Sn x | 0.1238 | 0.0013 | -0.1003 | -0.1161 | -0.1385 | -0.0164 |
| y | 0.0401 | 0.0194 | 0.0335 | -0.0671 | -0.0252 | 0.0024 |
| z | -0.0026 | -0.0248 | -0.0261 | -0.0466 | 0.0277 | -0.1039 |
| Sn x | -0.0048 | 0.0290 | 0.0738 | -0.0648 | 0.0139 | -0.0174 |
| y | 0.0432 | 0.0289 | 0.0930 | -0.1623 | 0.0450 | -0.0298 |
| z | -0.0345 | -0.0405 | -0.1135 | 0.1272 | -0.0573 | 0.0265 |
| Sn x | -0.0654 | -0.0337 | 0.1744 | -0.2037 | 0.0625 | -0.1617 |
| y | -0.0661 | -0.0238 | 0.0494 | -0.0668 | 0.0195 | -0.1932 |
| z | 0.0428 | -0.0080 | -0.0560 | 0.0893 | -0.0209 | 0.2074 |
| Ag x | 0.0099 | 0.1775 | -0.0493 | 0.1003 | -0.0107 | 0.0218 |
| y | -0.0623 | -0.0046 | -0.1176 | -0.0187 | 0.0039 | 0.0739 |
| z | 0.0914 | -0.0036 | -0.0306 | 0.0985 | -0.0625 | -0.0051 |
| Ag x | -0.0442 | 0.0807 | 0.1836 | 0.0312 | -0.0380 | 0.1307 |
| y | 0.1296 | 0.0121 | -0.0723 | -0.0594 | -0.0332 | -0.0126 |
| z | -0.2773 | -0.0322 | 0.0646 | 0.0878 | 0.0474 | -0.0524 |
| Ag x | 0.0759 | 0.0036 | -0.0607 | -0.0206 | 0.0361 | -0.0129 |
| y | 0.1362 | -0.0223 | -0.2398 | -0.2163 | 0.1783 | -0.0008 |
| z | 0.0806 | -0.0705 | -0.1491 | -0.0055 | 0.0791 | 0.0083 |
| Ag x | -0.0877 | -0.0236 | -0.1085 | 0.1532 | -0.1025 | 0.0237 |
| y | 0.0006 | -0.0074 | 0.0275 | -0.0003 | -0.0230 | -0.0001 |
| z | 0.0080 | -0.0074 | -0.0018 | -0.0246 | -0.0228 | -0.0003 |
| Ag x | -0.1085 | -0.0152 | 0.0835 | -0.0224 | -0.0102 | 0.0842 |
| y | 0.1981 | 0.0568 | 0.0162 | 0.0451 | -0.0110 | -0.0315 |
| z | 0.2052 | 0.0440 | 0.0103 | 0.0129 | -0.0073 | 0.0145 |
| Ag x | -0.0027 | -0.0472 | -0.3327 | 0.3461 | -0.1589 | 0.1308 |

| | | | | | | |
|---|---|---|---|---|---|---|
| y | -0.0529 | -0.0066 | 0.0349 | 0.0648 | 0.0497 | 0.0251 |
| z | -0.0737 | 0.0189 | 0.1539 | -0.0673 | 0.1014 | -0.0541 |
| Sn x | -0.2116 | -0.1147 | -0.2368 | -0.0017 | 0.0072 | -0.3869 |
| y | 0.0541 | 0.0276 | 0.0311 | -0.0132 | -0.0012 | 0.1654 |
| z | 0.1033 | 0.0794 | 0.1329 | 0.0057 | -0.0028 | 0.2714 |
| Sn x | -0.2116 | -0.0615 | 0.2101 | 0.3476 | 0.4850 | 0.0135 |
| y | -0.0968 | -0.0098 | -0.0353 | 0.1595 | 0.0355 | 0.0182 |
| z | 0.1367 | 0.0319 | -0.1436 | -0.0456 | -0.1409 | 0.0165 |
| Sn x | 0.1503 | 0.0741 | 0.1935 | 0.1875 | -0.0754 | -0.0358 |
| y | 0.0275 | -0.0918 | 0.2091 | 0.1771 | -0.0956 | -0.0168 |
| z | -0.0653 | 0.1225 | -0.0369 | 0.0622 | 0.0101 | -0.0015 |
| Sn x | 0.3048 | 0.1703 | 0.0850 | 0.2279 | -0.0924 | -0.3610 |
| y | 0.0464 | 0.0375 | 0.0622 | 0.0699 | -0.0305 | -0.1338 |
| z | -0.0649 | -0.0052 | -0.0338 | -0.0089 | 0.0022 | -0.0645 |
| Ag x | -0.2986 | -0.1926 | -0.2488 | -0.3130 | 0.1144 | 0.1212 |
| y | -0.1097 | -0.0117 | -0.0395 | -0.0229 | 0.0048 | 0.0263 |
| z | 0.0221 | 0.0052 | 0.0184 | 0.0175 | 0.0007 | -0.0045 |
| Ag x | 0.1045 | -0.0674 | -0.1083 | 0.0129 | 0.1148 | -0.0261 |
| y | 0.2288 | -0.0227 | -0.0576 | -0.0210 | 0.2764 | -0.0146 |
| z | -0.2663 | 0.1382 | 0.2001 | -0.0671 | -0.3184 | 0.0083 |
| Sn x | 0.0712 | 0.0721 | -0.1013 | -0.2474 | -0.3798 | -0.0068 |
| y | -0.0614 | -0.0256 | 0.0805 | -0.0802 | -0.2512 | -0.0062 |
| z | 0.1390 | -0.0911 | -0.0234 | 0.0500 | 0.2009 | -0.0064 |
| Ag x | 0.1124 | 0.0806 | 0.2561 | -0.3174 | 0.1731 | -0.0533 |
| y | -0.0870 | -0.1491 | -0.1587 | 0.1637 | -0.1238 | 0.0284 |
| z | -0.0202 | -0.0295 | 0.0731 | -0.1958 | 0.0310 | -0.0173 |
| Sn x | 0.0953 | -0.5702 | 0.1333 | -0.0118 | -0.0749 | -0.0045 |
| y | 0.0641 | 0.0562 | 0.0751 | -0.0504 | 0.0384 | -0.0109 |
| z | -0.0195 | 0.1594 | 0.0051 | -0.0496 | 0.0450 | -0.0041 |
| Ag x | 0.0305 | 0.0279 | 0.0103 | -0.0003 | -0.0559 | -0.0092 |
| y | -0.3011 | 0.0566 | 0.2227 | 0.0661 | -0.1665 | 0.0257 |
| z | 0.0921 | -0.0321 | -0.0624 | -0.0002 | 0.0663 | -0.0084 |
| Sn x | 0.0303 | -0.0153 | 0.0667 | -0.0855 | 0.0496 | 0.5809 |
| y | -0.0678 | -0.0579 | -0.1029 | 0.0114 | 0.0098 | 0.0791 |
| z | -0.1655 | -0.0853 | -0.0573 | -0.0872 | 0.0283 | -0.2328 |
| Sn x | -0.0940 | 0.4273 | -0.1232 | -0.0161 | 0.0633 | 0.0012 |
| y | -0.0173 | 0.0149 | -0.0566 | -0.0182 | -0.0179 | 0.0045 |
| z | 0.1279 | -0.3710 | 0.1742 | 0.0391 | -0.1095 | -0.0042 |
| Ag x | 0.0112 | -0.0019 | -0.0189 | 0.0131 | 0.0213 | 0.0035 |
| y | -0.0445 | 0.1244 | -0.0762 | 0.0412 | 0.1312 | 0.0073 |
| z | -0.0690 | 0.2132 | -0.0895 | 0.0017 | 0.1033 | 0.0014 |

STANDARD THERMODYNAMIC QUANTITIES AT 298.15 K AND 1.00 ATM

Zero point vibrational energy: 6.903 kcal/mol

Atom 1 Element Sn Has Mass 118.69000
Atom 2 Element Sn Has Mass 118.69000
Atom 3 Element Sn Has Mass 118.69000
Atom 4 Element Ag Has Mass 107.86800
Atom 5 Element Ag Has Mass 107.86800
Atom 6 Element Ag Has Mass 107.86800

```
Atom    7 Element Ag Has Mass  107.86800
Atom    8 Element Ag Has Mass  107.86800
Atom    9 Element Ag Has Mass  107.86800
Atom   10 Element Sn Has Mass  118.69000
Atom   11 Element Sn Has Mass  118.69000
Atom   12 Element Sn Has Mass  118.69000
Atom   13 Element Sn Has Mass  118.69000
Atom   14 Element Ag Has Mass  107.86800
Atom   15 Element Ag Has Mass  107.86800
Atom   16 Element Sn Has Mass  118.69000
Atom   17 Element Ag Has Mass  107.86800
Atom   18 Element Sn Has Mass  118.69000
Atom   19 Element Ag Has Mass  107.86800
Atom   20 Element Sn Has Mass  118.69000
Atom   21 Element Sn Has Mass  118.69000
Atom   22 Element Ag Has Mass  107.86800
Molecular Mass:  2492.138000 amu
Principal axes and moments of inertia in atomic units:
                      1            2            3
 Eigenvalues --     59101.40921   98973.01322  101763.23805
      X              0.90338      0.06547     -0.42382
      Y              0.31484     -0.77229      0.55177
      Z             -0.29119     -0.63189     -0.71828
Rotational Symmetry Number is   1
The Molecule is an Asymmetric Top
Symmetry Point Group c1


H,Trans:              0.889 kcal/mol
H,Rot  :              0.889 kcal/mol
H,pV   :              0.592 kcal/mol
H,Vib - ZPVE:        29.198 kcal/mol
S,Trans:             49.303  cal/mol.K
S,Rot  :             41.605  cal/mol.K   with Symmetry Number:   1
S,Vib  :            249.872  cal/mol.K
C,Trans:              4.968  cal/mol.K
C,Rot  :              2.981  cal/mol.K
C,Vib  :            117.401  cal/mol.K
===================================
H,Total - ZPVE:       31.568 kcal/mol
S,Total:            340.780  cal/mol.K
C,Total (p):        125.349  cal/mol.K
G,Total:            -70.036 kcal/mol
```

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```
STANDARD THERMODYNAMIC QUANTITIES
computed from     25.00 to   1000.00 in steps of   25.00

     T       Entropy   Heat_Capacity   Enthalpy   Free_Energy
    (K)        S  (cal/mol.K) Cp        H  (kcal/mol)  G
```

(ZPVE is included)

| | | | | | |
|---|---|---|---|---|---|
| 1 | 25.00 | 92.912 | 47.374 | 7.473 | 5.150 |
| 2 | 50.00 | 138.821 | 85.431 | 9.184 | 2.243 |
| 3 | 75.00 | 177.408 | 103.834 | 11.579 | -1.727 |
| 4 | 100.00 | 208.643 | 112.744 | 14.298 | -6.566 |
| 5 | 125.00 | 234.363 | 117.497 | 17.182 | -12.113 |
| 6 | 150.00 | 256.051 | 120.275 | 20.157 | -18.251 |
| 7 | 175.00 | 274.733 | 122.024 | 23.187 | -24.891 |
| 8 | 200.00 | 291.108 | 123.190 | 26.253 | -31.968 |
| 9 | 225.00 | 305.667 | 124.004 | 29.344 | -39.431 |
| 10 | 250.00 | 318.764 | 124.594 | 32.452 | -47.239 |
| 11 | 275.00 | 330.661 | 125.034 | 35.572 | -55.359 |
| 12 | 298.15 | 340.780 | 125.349 | 38.471 | -63.133 |
| 13 | 300.00 | 341.555 | 125.371 | 38.703 | -63.764 |
| 14 | 325.00 | 351.601 | 125.635 | 41.840 | -72.430 |
| 15 | 350.00 | 360.920 | 125.846 | 44.984 | -81.338 |
| 16 | 375.00 | 369.608 | 126.016 | 48.132 | -90.471 |
| 17 | 400.00 | 377.746 | 126.156 | 51.284 | -99.814 |
| 18 | 425.00 | 385.398 | 126.272 | 54.440 | -109.354 |
| 19 | 450.00 | 392.618 | 126.369 | 57.598 | -119.080 |
| 20 | 475.00 | 399.453 | 126.452 | 60.758 | -128.982 |
| 21 | 500.00 | 405.941 | 126.522 | 63.920 | -139.050 |
| 22 | 525.00 | 412.115 | 126.583 | 67.084 | -149.276 |
| 23 | 550.00 | 418.005 | 126.636 | 70.249 | -159.653 |
| 24 | 575.00 | 423.635 | 126.682 | 73.416 | -170.174 |
| 25 | 600.00 | 429.028 | 126.723 | 76.584 | -180.833 |
| 26 | 625.00 | 434.201 | 126.758 | 79.752 | -191.624 |
| 27 | 650.00 | 439.174 | 126.790 | 82.921 | -202.541 |
| 28 | 675.00 | 443.959 | 126.818 | 86.092 | -213.581 |
| 29 | 700.00 | 448.572 | 126.844 | 89.262 | -224.738 |
| 30 | 725.00 | 453.023 | 126.866 | 92.434 | -236.008 |
| 31 | 750.00 | 457.325 | 126.887 | 95.606 | -247.388 |
| 32 | 775.00 | 461.486 | 126.906 | 98.778 | -258.873 |
| 33 | 800.00 | 465.515 | 126.922 | 101.951 | -270.461 |
| 34 | 825.00 | 469.421 | 126.938 | 105.124 | -282.148 |
| 35 | 850.00 | 473.210 | 126.952 | 108.298 | -293.931 |
| 36 | 875.00 | 476.891 | 126.965 | 111.472 | -305.808 |
| 37 | 900.00 | 480.468 | 126.976 | 114.646 | -317.775 |
| 38 | 925.00 | 483.947 | 126.987 | 117.821 | -329.830 |
| 39 | 950.00 | 487.333 | 126.997 | 120.995 | -341.971 |
| 40 | 975.00 | 490.632 | 127.007 | 124.170 | -354.196 |
| 41 | 1000.00 | 493.848 | 127.015 | 127.346 | -366.502 |

Message: License checkin of MS_dmol successful

Message: DMol3 job finished successfully

time all done 0.01m 0.34s
Peak memory usage: 133044 kB on current thread

DMol3.pl message: DMol3 job finished in 1 hr 42 min 10 sec.