$coordinates

| | | | |
|---|---|---|---|
| Ag | -9.34003135457775 | 6.31898607074332 | -2.30550187933376 |
| Ag | 0.92208209658601 | 0.29416788520554 | 0.26488958734275 |
| Ag | -7.08608704885672 | 1.35910922715797 | -2.71823224364748 |
| Ag | -2.88511059592289 | 1.84815090491421 | -7.10888350674227 |
| Sn | -4.21961620876361 | -0.57436277261545 | 1.60123841258963 |
| Sn | -5.84205046609313 | 5.07393860922478 | 1.67546439624569 |
| Sn | -0.27810046426134 | 5.59566265622715 | 0.18087406646877 |
| Sn | 1.66396584363266 | -0.48536640988698 | -5.17373067116971 |
| Sn | 4.48049220301004 | 3.91836187137634 | -2.84438636676075 |
| Sn | 0.65361456982833 | 6.06465493317121 | -6.37034914807408 |
| Ag | -4.13633625055571 | 6.25454938997914 | -3.89010060143731 |
| Ag | -3.22426008750564 | -2.39255306759329 | -3.43261493489848 |

$end

vibrational frequencies, intensities

| mode | au_amu | cm-1 | km/mol |
|---|---|---|---|
| 7 | 0.004669 | 24.0 | 0.02 |
| 8 | 0.005706 | 29.3 | 0.05 |
| 9 | 0.007061 | 36.3 | 0.09 |
| 10 | 0.007689 | 39.5 | 0.04 |
| 11 | 0.008347 | 42.9 | 0.04 |
| 12 | 0.009131 | 46.9 | 0.11 |
| 13 | 0.009428 | 48.5 | 0.04 |
| 14 | 0.009676 | 49.7 | 0.04 |
| 15 | 0.010016 | 51.5 | 0.05 |
| 16 | 0.011388 | 58.5 | 0.01 |
| 17 | 0.012142 | 62.4 | 0.18 |
| 18 | 0.012422 | 63.9 | 0.05 |
| 19 | 0.014080 | 72.4 | 0.14 |
| 20 | 0.014542 | 74.8 | 0.04 |
| 21 | 0.015795 | 81.2 | 0.26 |
| 22 | 0.016191 | 83.2 | 0.11 |
| 23 | 0.017282 | 88.8 | 0.13 |
| 24 | 0.018577 | 95.5 | 0.06 |
| 25 | 0.019964 | 102.6 | 0.12 |
| 26 | 0.020880 | 107.3 | 0.08 |
| 27 | 0.021149 | 108.7 | 0.46 |
| 28 | 0.022732 | 116.9 | 0.05 |
| 29 | 0.023176 | 119.1 | 0.04 |
| 30 | 0.023639 | 121.5 | 0.43 |
| 31 | 0.025077 | 128.9 | 0.45 |
| 32 | 0.026059 | 134.0 | 0.34 |
| 33 | 0.026468 | 136.1 | 0.27 |
| 34 | 0.027557 | 141.7 | 0.07 |
| 35 | 0.028540 | 146.7 | 0.13 |
| 36 | 0.029467 | 151.5 | 0.71 |

Frequencies (cm-1) and normal modes

| | 7: 24.0 | 8: 29.3 | 9: 36.3 | 10: 39.5 | 11: 42.9 | 12: 46.9 | 13: 48.5 | 14: 49.7 | 15: 51.5 |
|---|---|---|---|---|---|---|---|---|---|
| Ag x | -0.1058 | 0.1252 | -0.1843 | 0.1989 | -0.1505 | -0.2552 | 0.0631 | 0.0728 | -0.0006 |
| y | -0.2219 | 0.1259 | -0.2090 | 0.2900 | 0.0416 | 0.2113 | 0.1929 | 0.0832 | -0.1742 |
| z | -0.3273 | 0.0909 | 0.1766 | -0.1720 | 0.2911 | 0.1070 | -0.1918 | 0.3195 | 0.0796 |
| Ag x | 0.1448 | -0.0713 | -0.2536 | -0.0927 | -0.0177 | 0.3430 | 0.2311 | -0.0142 | 0.3438 |
| y | -0.1436 | 0.1212 | -0.1890 | -0.3598 | -0.0639 | -0.1340 | 0.0819 | 0.1066 | -0.2848 |
| z | -0.1789 | 0.1076 | 0.1031 | -0.1391 | -0.1496 | -0.0098 | 0.0934 | -0.2400 | 0.3270 |
| Ag x | 0.1253 | 0.4173 | 0.0003 | -0.0465 | 0.3956 | -0.1504 | -0.0528 | -0.2959 | 0.1061 |
| y | -0.0978 | 0.2378 | -0.0415 | 0.0383 | 0.2614 | 0.1880 | 0.0571 | -0.1765 | 0.0356 |
| z | -0.0840 | -0.2869 | -0.3061 | 0.1305 | -0.2819 | 0.0868 | -0.2345 | -0.2510 | -0.1356 |
| Ag x | -0.2502 | -0.1745 | 0.1114 | -0.0642 | 0.1769 | 0.2644 | -0.0286 | -0.2219 | -0.2535 |
| y | 0.1393 | -0.0781 | -0.0183 | -0.1697 | -0.1468 | -0.0746 | -0.1960 | -0.1901 | 0.0322 |
| z | 0.3353 | 0.2615 | 0.1621 | 0.0469 | -0.3290 | 0.3210 | -0.0307 | 0.2492 | -0.2517 |
| Sn x | 0.1321 | -0.0579 | -0.3517 | -0.1566 | 0.0020 | 0.2026 | 0.1178 | -0.0284 | 0.1302 |
| y | 0.2454 | -0.2283 | 0.0547 | -0.0609 | 0.2410 | 0.0384 | 0.1312 | 0.2324 | 0.1746 |
| z | 0.0749 | -0.0915 | -0.0675 | 0.1488 | 0.1065 | -0.1791 | -0.1886 | -0.2458 | -0.0882 |
| Sn x | -0.1131 | -0.0455 | 0.3122 | -0.0967 | -0.1203 | -0.0779 | -0.1008 | 0.0607 | 0.0822 |
| y | 0.1533 | -0.2733 | 0.2287 | 0.0166 | 0.0987 | -0.0086 | 0.0151 | 0.1031 | 0.1715 |
| z | -0.1834 | 0.0821 | -0.1076 | 0.0314 | 0.1109 | -0.0822 | -0.0360 | 0.0624 | 0.0853 |
| Sn x | 0.0338 | -0.0579 | 0.2994 | -0.0539 | -0.1390 | -0.1475 | 0.1504 | -0.0399 | -0.0861 |
| y | -0.1095 | 0.1010 | -0.1443 | -0.3718 | -0.0195 | -0.1975 | 0.0393 | 0.1586 | -0.2880 |
| z | 0.1809 | -0.0520 | -0.1202 | 0.1131 | 0.1249 | -0.1016 | 0.3942 | 0.0095 | -0.0730 |
| Sn x | -0.1035 | -0.0615 | 0.1240 | 0.2215 | 0.0614 | 0.2642 | -0.0557 | 0.1721 | -0.2266 |
| y | -0.0022 | -0.0045 | 0.0553 | 0.1877 | -0.1550 | -0.2921 | -0.0456 | 0.1194 | 0.2705 |
| z | -0.2730 | 0.1233 | 0.1780 | -0.1176 | -0.2015 | 0.0984 | 0.1350 | -0.1583 | 0.1825 |
| Sn x | 0.0012 | -0.0972 | 0.1573 | -0.0893 | -0.1496 | -0.0159 | -0.0045 | 0.0455 | -0.0172 |
| y | -0.1776 | 0.1025 | 0.1239 | 0.3629 | -0.1690 | 0.0711 | 0.1429 | 0.0390 | 0.1532 |
| z | -0.0015 | -0.0290 | -0.2372 | -0.0313 | 0.0490 | -0.0199 | -0.2780 | 0.3479 | 0.2052 |
| Sn x | 0.0092 | -0.0716 | -0.1416 | -0.1353 | -0.0933 | -0.0646 | -0.2355 | 0.0921 | 0.0471 |
| y | 0.0303 | -0.1179 | 0.1255 | -0.0482 | 0.0195 | -0.0392 | 0.0446 | -0.2871 | -0.1369 |
| z | 0.1593 | -0.2277 | 0.0698 | -0.1972 | 0.1099 | 0.0446 | 0.0797 | -0.0326 | -0.0851 |
| Ag x | 0.0161 | 0.0835 | -0.1423 | 0.1094 | -0.1369 | -0.2501 | 0.1049 | 0.0344 | 0.0006 |
| y | 0.3293 | 0.3528 | 0.0454 | -0.0335 | -0.1503 | 0.2281 | -0.3341 | -0.1291 | 0.0153 |
| z | 0.1312 | -0.0170 | 0.0993 | -0.0059 | -0.0283 | -0.1230 | 0.3497 | 0.0163 | -0.1655 |
| Ag x | 0.1121 | 0.0307 | 0.0495 | 0.2204 | 0.1928 | -0.1204 | -0.1830 | 0.1079 | -0.1227 |
| y | -0.1517 | -0.3186 | -0.0532 | 0.1442 | 0.0416 | 0.0302 | -0.1454 | -0.0775 | 0.0143 |
| z | 0.1685 | 0.0483 | 0.0637 | 0.1950 | 0.1831 | -0.1305 | -0.0976 | -0.0763 | -0.0916 |

| | 16: 58.5 | 17: 62.4 | 18: 63.9 | 19: 72.4 | 20: 74.8 | 21: 81.2 | 22: 83.2 | 23: 88.8 | 24: 95.5 |
|---|---|---|---|---|---|---|---|---|---|
| Ag x | 0.0996 | -0.3336 | 0.0573 | 0.2867 | 0.1348 | 0.2331 | -0.1912 | 0.0656 | -0.1981 |
| y | -0.3686 | -0.1219 | 0.0210 | 0.1797 | -0.1024 | -0.0894 | 0.2407 | -0.1705 | -0.1287 |
| z | 0.0752 | -0.0664 | 0.0830 | 0.0083 | 0.0870 | -0.3256 | 0.1724 | 0.1314 | -0.0569 |
| Ag x | -0.1067 | -0.0457 | 0.1913 | -0.0046 | 0.0082 | 0.0194 | 0.0096 | -0.0482 | 0.0910 |
| y | -0.0475 | 0.0623 | 0.0464 | 0.0406 | 0.0246 | 0.0104 | 0.0143 | 0.1709 | -0.0391 |
| z | -0.1036 | 0.0604 | 0.2148 | 0.2914 | -0.1444 | -0.1728 | -0.1024 | 0.0204 | 0.2610 |
| Ag x | -0.0097 | 0.0746 | -0.3242 | -0.0177 | -0.2205 | 0.0240 | -0.0635 | 0.0336 | -0.2377 |
| y | -0.1342 | 0.2111 | -0.1137 | -0.3142 | -0.0711 | 0.0270 | -0.2049 | 0.0331 | 0.2430 |
| z | 0.0169 | 0.1032 | -0.3739 | 0.1201 | -0.1637 | -0.0617 | 0.1556 | 0.1214 | 0.1513 |
| Ag x | 0.2834 | -0.2152 | 0.0034 | -0.0612 | 0.0697 | 0.0525 | 0.1983 | -0.1183 | 0.1058 |
| y | 0.1007 | -0.0413 | 0.1941 | 0.0232 | -0.2481 | -0.2084 | 0.0474 | -0.3175 | -0.4358 |
| z | -0.0022 | -0.1567 | -0.0205 | -0.1505 | -0.2472 | -0.1186 | -0.3822 | 0.0421 | -0.0493 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.0248 | -0.0167 | -0.0421 | -0.0627 | 0.0967 | -0.0079 | -0.0294 | -0.1389 | -0.0636 |
| y | 0.1910 | -0.1468 | 0.1098 | 0.0409 | -0.0390 | 0.0623 | 0.0355 | 0.0614 | -0.0782 |
| z | -0.0085 | 0.0017 | 0.0293 | -0.1634 | 0.1531 | -0.0099 | -0.0224 | -0.0650 | -0.2807 |
| Sn x | -0.1150 | 0.0005 | -0.1966 | 0.1071 | 0.2494 | 0.0464 | -0.2466 | -0.3484 | 0.0847 |
| y | 0.1855 | -0.0022 | -0.3322 | 0.1824 | -0.2155 | -0.0077 | 0.0465 | 0.0629 | 0.0290 |
| z | 0.2501 | -0.1258 | 0.0792 | 0.0127 | -0.2170 | 0.4159 | -0.1371 | 0.1973 | 0.0680 |
| Sn x | -0.0961 | 0.1685 | -0.0622 | -0.0462 | 0.1215 | -0.0873 | 0.0208 | -0.0999 | 0.0521 |
| y | 0.0032 | 0.0925 | -0.0741 | 0.0135 | 0.0660 | 0.0246 | -0.0619 | -0.1445 | 0.0860 |
| z | 0.1673 | 0.1636 | -0.1286 | 0.1111 | 0.3252 | -0.4468 | -0.0836 | 0.1835 | -0.0591 |
| Sn x | 0.0733 | 0.1766 | -0.0322 | 0.0223 | -0.0304 | 0.0622 | -0.0975 | 0.0507 | -0.0459 |
| y | -0.2533 | -0.0232 | -0.0711 | -0.1755 | -0.0248 | 0.0042 | 0.1545 | 0.1249 | 0.1522 |
| z | 0.0685 | 0.0235 | 0.0393 | 0.0283 | 0.0067 | 0.0218 | 0.0587 | 0.0006 | -0.2590 |
| Sn x | -0.2452 | 0.0985 | 0.0839 | -0.2241 | -0.0893 | 0.1533 | 0.2382 | 0.3958 | -0.1860 |
| y | 0.1263 | -0.0242 | -0.1670 | -0.1644 | 0.1469 | 0.0119 | 0.0944 | -0.0665 | -0.1860 |
| z | -0.0505 | 0.0186 | -0.2213 | -0.0704 | 0.0746 | 0.1008 | -0.0239 | -0.3648 | 0.1021 |
| Sn x | 0.0423 | -0.0740 | 0.0531 | -0.2830 | -0.1072 | -0.2435 | 0.0774 | 0.1399 | 0.0410 |
| y | -0.0379 | -0.5140 | -0.0299 | -0.0083 | -0.0310 | -0.0924 | -0.1871 | 0.0520 | 0.2830 |
| z | -0.4054 | -0.0667 | -0.1315 | 0.1387 | 0.1649 | 0.2943 | -0.0205 | 0.1918 | -0.1286 |
| Ag x | 0.2785 | 0.0010 | 0.0682 | -0.1434 | 0.0116 | -0.1124 | 0.0426 | 0.0959 | 0.2329 |
| y | 0.1972 | 0.1482 | 0.0873 | 0.2466 | 0.4065 | 0.1868 | 0.2684 | 0.1302 | 0.1393 |
| z | 0.1784 | 0.2577 | 0.1321 | -0.0911 | -0.2572 | 0.2917 | 0.2643 | -0.3267 | 0.1321 |
| Ag x | -0.1616 | 0.1483 | 0.2097 | 0.4506 | -0.2563 | -0.1361 | 0.0430 | -0.0278 | 0.1296 |
| y | 0.0271 | 0.3898 | 0.3571 | -0.0592 | 0.0927 | 0.0707 | -0.4516 | 0.0592 | -0.0787 |
| z | -0.1873 | -0.2139 | 0.3145 | -0.2380 | 0.1930 | -0.0075 | 0.1324 | -0.1389 | 0.1463 |

25: 102.6 26: 107.3 27: 108.7 28: 116.9 29: 119.1 30: 121.5 31: 128.9 32: 134.0 33: 136.1

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Ag x | 0.0301 | -0.0708 | 0.0599 | 0.0914 | -0.0245 | 0.2746 | 0.0106 | 0.2584 | -0.0572 |
| y | 0.1208 | -0.0047 | 0.0351 | -0.0412 | 0.0966 | -0.2138 | 0.0151 | -0.1402 | -0.0432 |
| z | 0.1538 | -0.1451 | -0.0837 | 0.1218 | 0.0114 | 0.1466 | -0.0136 | 0.0984 | -0.0401 |
| Ag x | -0.1686 | -0.1529 | 0.0933 | 0.3524 | 0.0705 | -0.0166 | 0.4061 | 0.0198 | 0.2302 |
| y | -0.2552 | -0.4137 | 0.0209 | -0.4192 | -0.0017 | -0.0255 | 0.1608 | 0.0543 | -0.0348 |
| z | 0.1906 | -0.1424 | 0.3160 | -0.0212 | -0.2905 | -0.0281 | -0.1727 | -0.0708 | -0.1486 |
| Ag x | 0.1506 | -0.0965 | 0.0062 | 0.0313 | 0.0860 | 0.0928 | 0.2218 | -0.0524 | -0.2205 |
| y | -0.1990 | 0.1072 | -0.0616 | -0.0646 | -0.1810 | 0.1933 | -0.1357 | 0.1237 | 0.2356 |
| z | -0.0082 | 0.1042 | -0.0884 | -0.0227 | -0.1245 | 0.2593 | 0.1884 | 0.0171 | -0.0654 |
| Ag x | -0.0420 | 0.0268 | 0.3749 | -0.0832 | 0.2717 | 0.2523 | -0.0432 | -0.1217 | 0.0200 |
| y | -0.2634 | 0.0827 | 0.1050 | 0.0228 | -0.2263 | 0.1027 | -0.0827 | 0.1613 | 0.0636 |
| z | 0.0631 | -0.0260 | 0.1310 | -0.0162 | 0.1899 | 0.1421 | -0.0144 | -0.1046 | -0.0133 |
| Sn x | 0.1687 | 0.1152 | -0.1087 | -0.2661 | 0.1176 | -0.1073 | -0.5588 | 0.1175 | -0.2088 |
| y | 0.2680 | 0.2655 | -0.0493 | -0.3030 | -0.2902 | 0.2228 | 0.2168 | -0.1791 | 0.0398 |
| z | 0.2902 | -0.1784 | 0.1739 | 0.0178 | -0.0075 | -0.2995 | -0.0273 | -0.1184 | 0.4213 |
| Sn x | -0.1807 | -0.0748 | -0.0441 | -0.2336 | -0.0344 | -0.0052 | 0.0300 | -0.1999 | 0.2833 |
| y | -0.2039 | -0.2732 | 0.0334 | 0.2175 | 0.2429 | -0.1801 | -0.2444 | 0.1965 | -0.0553 |
| z | -0.2796 | 0.2912 | 0.1681 | -0.0549 | -0.0098 | -0.3522 | -0.0503 | -0.1612 | -0.0243 |
| Sn x | 0.0448 | 0.2590 | 0.1261 | 0.0108 | -0.0312 | -0.1358 | 0.2053 | 0.0383 | -0.3902 |
| y | 0.1401 | 0.3305 | 0.0827 | 0.5371 | -0.0044 | 0.0109 | -0.0763 | -0.0541 | 0.0850 |
| z | -0.2116 | 0.1479 | 0.1484 | -0.0795 | 0.0612 | -0.0853 | 0.0627 | 0.0304 | 0.0645 |
| Sn x | 0.1407 | -0.0294 | 0.0484 | 0.0179 | -0.4147 | -0.1913 | -0.0185 | 0.4352 | 0.1080 |
| y | 0.1727 | 0.1165 | 0.3160 | -0.1558 | 0.2847 | 0.1818 | -0.0499 | 0.1803 | 0.1984 |
| z | -0.0090 | 0.2731 | -0.4555 | -0.0560 | 0.2915 | -0.0104 | 0.0660 | 0.1800 | 0.1791 |
| Sn x | -0.0520 | 0.0589 | 0.0385 | 0.0160 | -0.0447 | -0.1186 | 0.0393 | 0.0601 | 0.0061 |
| y | -0.1562 | -0.1068 | -0.0941 | 0.1412 | -0.2317 | 0.0252 | -0.0707 | -0.3820 | -0.1943 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| z | 0.0166 | -0.0350 | -0.0288 | -0.0690 | -0.0001 | -0.1014 | 0.2099 | 0.1153 | -0.1467 |
| Sn x | -0.0474 | -0.0230 | -0.1037 | 0.0278 | -0.0270 | -0.1797 | -0.0271 | -0.3040 | -0.0705 |
| y | 0.1778 | -0.0275 | -0.3036 | 0.0003 | -0.0135 | -0.2922 | 0.1748 | 0.1256 | -0.0268 |
| z | -0.0220 | -0.1059 | -0.1145 | 0.1562 | -0.1214 | 0.2210 | -0.2352 | -0.2026 | 0.0034 |
| Ag x | 0.1028 | -0.1872 | -0.2698 | 0.0987 | -0.0729 | 0.1409 | -0.1795 | -0.0748 | 0.1610 |
| y | 0.0639 | 0.0094 | -0.0035 | -0.0094 | 0.0330 | -0.1136 | 0.0130 | -0.0090 | -0.0114 |
| z | 0.1511 | -0.2265 | -0.1037 | -0.0410 | 0.0389 | 0.0362 | 0.0335 | 0.0129 | 0.0090 |
| Ag x | -0.1507 | 0.1599 | -0.2189 | -0.0424 | 0.1249 | 0.0302 | -0.0697 | -0.1837 | 0.1518 |
| y | 0.1149 | -0.1009 | -0.0802 | 0.0530 | 0.2922 | 0.0899 | 0.0815 | -0.0717 | -0.2590 |
| z | -0.3246 | 0.0237 | -0.0575 | 0.0689 | -0.0497 | 0.1024 | -0.0483 | 0.2110 | -0.2633 |

34: 141.7 35: 146.7 36: 151.5

| | | | |
|---|---|---|---|
| Ag x | 0.0004 | -0.2835 | -0.2781 |
| y | 0.0827 | 0.1474 | 0.1186 |
| z | -0.0629 | -0.0591 | -0.0209 |
| Ag x | -0.0816 | 0.0847 | -0.0360 |
| y | -0.1573 | 0.0837 | -0.0391 |
| z | 0.0757 | -0.0846 | 0.0441 |
| Ag x | 0.1857 | 0.1533 | 0.1060 |
| y | -0.1864 | -0.2582 | -0.1807 |
| z | 0.0755 | 0.0098 | 0.0064 |
| Ag x | -0.0618 | -0.0517 | 0.0654 |
| y | -0.0572 | 0.0862 | 0.1121 |
| z | -0.0460 | -0.0187 | 0.0540 |
| Sn x | 0.0066 | -0.0727 | 0.0112 |
| y | 0.0240 | 0.0050 | 0.0203 |
| z | -0.2492 | -0.1249 | -0.0830 |
| Sn x | 0.3389 | 0.0609 | 0.1088 |
| y | -0.0344 | -0.0246 | -0.0290 |
| z | -0.0482 | 0.1911 | 0.0772 |
| Sn x | -0.5264 | 0.1025 | -0.1397 |
| y | 0.1676 | -0.0400 | 0.0451 |
| z | 0.2108 | -0.0881 | 0.0398 |
| Sn x | 0.1318 | 0.3078 | -0.0752 |
| y | 0.0473 | 0.2369 | -0.1033 |
| z | -0.0303 | 0.1238 | -0.0817 |
| Sn x | 0.1758 | -0.4721 | 0.3883 |
| y | -0.0594 | -0.1367 | -0.0390 |
| z | -0.1696 | -0.2075 | 0.1913 |
| Sn x | 0.2308 | 0.0851 | -0.5460 |
| y | 0.0264 | -0.1412 | 0.0494 |
| z | -0.1367 | 0.2465 | -0.0682 |
| Ag x | -0.2293 | 0.2761 | 0.4622 |
| y | 0.0347 | 0.0036 | -0.0308 |
| z | 0.1949 | -0.1344 | -0.2164 |
| Ag x | -0.1885 | -0.1909 | -0.0544 |
| y | 0.1035 | 0.0429 | 0.0791 |
| z | 0.2068 | 0.1393 | 0.0536 |