$coordinates

| | | | |
|---|---|---|---|
| Sn | 0.93411959908989 | 0.47509626429287 | 0.80196589599622 |
| Sn | 2.72483043973140 | 5.02208584338379 | -1.95057091071542 |
| Ag | -3.26483300251750 | -0.95565214767181 | -3.40321035986684 |
| Ag | 1.51209897491678 | -3.36772389972316 | -3.04525366193264 |
| Ag | -4.42113731138023 | 1.53584873916116 | 1.20008804430548 |
| Ag | -3.31465715303249 | 2.53359589687002 | -7.47284191626795 |
| Sn | 1.79805838116413 | 1.23995378978629 | -5.98578714342473 |
| Sn | -2.83397329740036 | 5.07952076193225 | -2.65252324618814 |

$end

vibrational frequencies, intensities

| mode | au_amu | cm-1 | km/mol |
|---|---|---|---|
| 7 | 0.003798 | 19.5 | 0.05 |
| 8 | 0.004445 | 22.8 | 0.05 |
| 9 | 0.009239 | 47.5 | 0.01 |
| 10 | 0.010849 | 55.8 | 0.23 |
| 11 | 0.010910 | 56.1 | 0.23 |
| 12 | 0.013957 | 71.7 | 0.00 |
| 13 | 0.016753 | 86.1 | 0.22 |
| 14 | 0.018018 | 92.6 | 0.02 |
| 15 | 0.018237 | 93.7 | 0.01 |
| 16 | 0.019355 | 99.5 | 0.00 |
| 17 | 0.020318 | 104.4 | 0.01 |
| 18 | 0.020336 | 104.5 | 0.01 |
| 19 | 0.024682 | 126.9 | 0.09 |
| 20 | 0.025100 | 129.0 | 0.46 |
| 21 | 0.025451 | 130.8 | 0.46 |
| 22 | 0.026816 | 137.8 | 0.19 |
| 23 | 0.026974 | 138.7 | 0.23 |
| 24 | 0.030053 | 154.5 | 0.04 |

Frequencies (cm-1) and normal modes

| | 7: 19.5 | 8: 22.8 | 9: 47.5 | 10: 55.8 | 11: 56.1 | 12: 71.7 | 13: 86.1 | 14: 92.6 | 15: 93.7 |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | -0.2473 | 0.0579 | -0.1079 | 0.1644 | 0.1108 | 0.0270 | -0.1978 | 0.4637 | -0.0322 |
| y | -0.0962 | 0.2197 | -0.1391 | -0.1153 | -0.1752 | 0.2163 | 0.0495 | 0.0198 | -0.1378 |
| z | 0.0025 | 0.0992 | 0.0349 | -0.1640 | 0.2902 | -0.1836 | -0.3357 | 0.3344 | -0.2587 |
| Sn x | 0.1546 | 0.0812 | -0.1308 | -0.2512 | 0.0465 | 0.3373 | 0.1542 | -0.0403 | -0.0543 |
| y | -0.1744 | -0.0204 | -0.1548 | 0.2370 | -0.1296 | 0.3085 | 0.1676 | 0.0658 | 0.0318 |
| z | 0.0861 | -0.2358 | -0.0365 | 0.1289 | 0.3191 | 0.0808 | 0.0506 | -0.0624 | 0.0897 |
| Ag x | 0.2724 | 0.1433 | 0.5251 | 0.2271 | -0.0519 | 0.1645 | -0.2211 | 0.0166 | 0.0244 |
| y | -0.2744 | -0.0541 | 0.5375 | -0.1155 | 0.0882 | 0.1827 | -0.2252 | -0.0194 | -0.0195 |
| z | 0.1191 | -0.3729 | 0.1177 | -0.0731 | -0.2539 | 0.0410 | -0.0651 | 0.0043 | -0.0653 |
| Ag x | 0.3727 | 0.0498 | 0.2030 | -0.1135 | 0.0030 | -0.2698 | 0.3381 | -0.0944 | -0.1562 |
| y | 0.0244 | -0.0603 | -0.1773 | -0.5464 | 0.1917 | -0.2608 | -0.0870 | 0.0627 | -0.0151 |
| z | -0.1029 | 0.4683 | 0.0190 | -0.0342 | 0.1741 | -0.0567 | 0.0499 | -0.2369 | 0.3857 |
| Ag x | -0.2734 | -0.0223 | -0.1452 | 0.2929 | 0.3813 | -0.2907 | 0.0185 | -0.2979 | -0.0256 |
| y | 0.2863 | -0.3248 | 0.0591 | 0.2420 | 0.0466 | -0.2855 | 0.2177 | 0.3367 | 0.1457 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| z | -0.2938 | -0.2211 | 0.2762 | -0.1921 | -0.0807 | -0.0309 | 0.2738 | -0.2642 | 0.0974 |
| Ag x | -0.3364 | -0.1555 | -0.0846 | -0.0535 | -0.4077 | -0.2777 | 0.0521 | -0.0740 | -0.2903 |
| y | -0.0542 | 0.4115 | 0.1368 | 0.0950 | -0.1555 | -0.2893 | 0.2719 | 0.1603 | 0.1705 |
| z | 0.2807 | 0.0837 | -0.2840 | 0.1117 | -0.3358 | -0.0979 | -0.2247 | -0.0301 | 0.2436 |
| Sn x | -0.1386 | -0.1935 | -0.0936 | -0.0283 | -0.2027 | -0.0048 | -0.2786 | 0.0125 | 0.4998 |
| y | 0.0777 | -0.2355 | -0.1304 | -0.0309 | 0.1863 | 0.1764 | -0.0138 | -0.0982 | 0.1806 |
| z | -0.0874 | -0.0084 | -0.0906 | 0.3155 | 0.0932 | 0.2030 | 0.2753 | 0.0989 | -0.3074 |
| Sn x | 0.1976 | 0.0398 | -0.1427 | -0.2214 | 0.1172 | 0.2826 | 0.1433 | -0.0071 | 0.0134 |
| y | 0.2100 | 0.0625 | -0.1058 | 0.2188 | -0.0446 | -0.0789 | -0.3723 | -0.5024 | -0.3430 |
| z | -0.0040 | 0.1850 | -0.0306 | -0.1014 | -0.2294 | 0.0374 | -0.0226 | 0.1314 | -0.1541 |

16: 99.5 17: 104.4 18: 104.5 19: 126.9 20: 129.0 21: 130.8 22: 137.8 23: 138.7 24: 154.5

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.2457 | -0.1960 | -0.2698 | -0.2269 | -0.0036 | 0.2153 | -0.2880 | -0.0491 | 0.1374 |
| y | -0.2501 | 0.0471 | 0.2641 | -0.0490 | 0.2370 | 0.4020 | 0.1083 | 0.2509 | 0.3274 |
| z | -0.2466 | -0.0414 | 0.2627 | -0.2520 | -0.0813 | -0.3068 | 0.0294 | 0.2324 | -0.1910 |
| Sn x | -0.0015 | -0.0134 | 0.0615 | -0.0045 | -0.2994 | 0.3225 | 0.0369 | 0.0904 | -0.5356 |
| y | -0.0181 | 0.0207 | -0.0652 | -0.0422 | 0.2241 | -0.4028 | -0.0432 | -0.1010 | -0.5110 |
| z | 0.0096 | -0.0937 | -0.0208 | -0.0517 | 0.5167 | 0.3751 | -0.0960 | 0.0436 | -0.0869 |
| Ag x | -0.0033 | -0.0180 | 0.4092 | 0.2368 | -0.0068 | 0.0441 | -0.1354 | -0.2843 | -0.0019 |
| y | -0.0016 | 0.1639 | -0.3947 | 0.2616 | 0.0381 | -0.0409 | 0.0198 | 0.3142 | -0.0037 |
| z | 0.0110 | -0.5609 | -0.1178 | 0.0854 | 0.0470 | 0.0019 | 0.4252 | -0.1104 | -0.0054 |
| Ag x | -0.0267 | 0.1001 | -0.3802 | -0.1835 | 0.0034 | -0.0230 | 0.0657 | 0.2663 | 0.0072 |
| y | -0.0523 | 0.0396 | -0.0835 | 0.3482 | -0.0082 | 0.1014 | -0.1312 | -0.4727 | -0.0472 |
| z | 0.3912 | -0.1146 | -0.0997 | 0.0226 | -0.0533 | -0.0278 | 0.0069 | -0.0263 | -0.0072 |
| Ag x | -0.1500 | 0.0790 | 0.1692 | 0.2726 | 0.0930 | -0.0387 | 0.3189 | 0.0740 | -0.0392 |
| y | 0.1820 | 0.2760 | 0.1266 | -0.0189 | 0.0066 | 0.0449 | -0.0290 | 0.0043 | -0.0089 |
| z | -0.1530 | 0.1210 | 0.2045 | -0.3231 | -0.0833 | -0.0074 | -0.3983 | -0.1150 | 0.0361 |
| Ag x | 0.2775 | -0.1278 | 0.1612 | 0.1863 | 0.0282 | -0.0519 | -0.1861 | 0.1450 | -0.0248 |
| y | -0.2268 | -0.3649 | 0.0241 | -0.0806 | -0.0367 | 0.0054 | 0.1128 | -0.0852 | -0.0024 |
| z | -0.1944 | 0.0795 | -0.1054 | 0.3495 | -0.0260 | -0.0439 | -0.3509 | 0.3267 | -0.0295 |
| Sn x | -0.2823 | 0.2369 | -0.1191 | -0.2666 | -0.1253 | 0.0287 | 0.2844 | -0.1444 | 0.0616 |
| y | 0.3131 | -0.1736 | 0.2578 | -0.0369 | -0.4216 | -0.1239 | 0.0534 | 0.2884 | 0.2361 |
| z | -0.2345 | 0.1118 | -0.2181 | 0.2149 | -0.4433 | 0.0223 | -0.0028 | -0.2146 | 0.2447 |
| Sn x | -0.0549 | -0.0592 | -0.0153 | 0.0097 | 0.3159 | -0.5002 | -0.0935 | -0.0885 | 0.3926 |
| y | 0.0492 | -0.0034 | -0.1444 | -0.3583 | -0.0394 | 0.0190 | -0.0923 | -0.2102 | 0.0068 |
| z | 0.4193 | 0.4760 | 0.0891 | -0.0393 | 0.1181 | -0.0169 | 0.3717 | -0.1329 | 0.0390 |