$coordinates

| | | | |
|---|---|---|---|
| Ag | -0.71852518823549 | 1.71495522573248 | -0.90713689139086 |
| Ag | -2.50065986779641 | -5.37749277543151 | -1.51824627289864 |
| Ag | 3.97932961590794 | 0.46923274081402 | -4.21998455040045 |
| Ag | 2.25042849861138 | -4.02821998471443 | 4.75369102194905 |
| Ag | 2.49070648187482 | -3.19479737127032 | -0.43890997242469 |
| Sn | -2.91521905425184 | -1.90531242733554 | -8.80305904889130 |
| Sn | -0.45896013290677 | 2.59329549911147 | -6.32641402478173 |
| Sn | -2.37739039271568 | -1.95802481825243 | 2.88230700391303 |
| Sn | -4.84668234885371 | -0.93281237348402 | -3.50750237183116 |
| Sn | 1.16277390530439 | -4.07744872032195 | -5.71341653664425 |

$end

vibrational frequencies, intensities

| mode | au_amu | cm-1 | km/mol |
|---|---|---|---|
| 7 | 0.002670 | 13.7 | 0.02 |
| 8 | 0.004241 | 21.8 | 0.09 |
| 9 | 0.005701 | 29.3 | 0.03 |
| 10 | 0.007687 | 39.5 | 0.06 |
| 11 | 0.008555 | 44.0 | 0.11 |
| 12 | 0.009786 | 50.3 | 0.08 |
| 13 | 0.010418 | 53.6 | 0.05 |
| 14 | 0.010674 | 54.9 | 0.04 |
| 15 | 0.012436 | 63.9 | 0.04 |
| 16 | 0.013218 | 67.9 | 0.17 |
| 17 | 0.013378 | 68.8 | 0.02 |
| 18 | 0.014917 | 76.7 | 0.02 |
| 19 | 0.018320 | 94.2 | 0.03 |
| 20 | 0.018575 | 95.5 | 0.14 |
| 21 | 0.020345 | 104.6 | 0.04 |
| 22 | 0.020719 | 106.5 | 0.11 |
| 23 | 0.021759 | 111.9 | 0.14 |
| 24 | 0.022400 | 115.1 | 0.08 |
| 25 | 0.022702 | 116.7 | 0.14 |
| 26 | 0.024217 | 124.5 | 0.11 |
| 27 | 0.025538 | 131.3 | 0.67 |
| 28 | 0.026647 | 137.0 | 0.03 |
| 29 | 0.028719 | 147.6 | 0.11 |
| 30 | 0.030594 | 157.3 | 1.73 |

Frequencies (cm-1) and normal modes

| | 7: 13.7 | 8: 21.8 | 9: 29.3 | 10: 39.5 | 11: 44.0 | 12: 50.3 | 13: 53.6 | 14: 54.9 | 15: 63.9 |
|---|---|---|---|---|---|---|---|---|---|
| Ag x | 0.0122 | -0.2625 | 0.2406 | 0.1475 | -0.4191 | -0.0423 | -0.2993 | -0.1593 | 0.1196 |
| y | 0.1154 | -0.0884 | -0.0150 | -0.0384 | 0.5406 | -0.0084 | 0.0918 | -0.4003 | -0.1774 |
| z | -0.1016 | -0.0091 | -0.0766 | -0.0692 | -0.0937 | -0.2194 | 0.2363 | -0.3256 | 0.0705 |
| Ag x | 0.0772 | -0.3338 | -0.0621 | 0.0973 | 0.0929 | 0.2219 | 0.2811 | 0.1074 | 0.2571 |
| y | 0.1324 | 0.2838 | 0.0893 | -0.0277 | -0.1827 | -0.0279 | 0.4238 | 0.0962 | 0.1474 |
| z | 0.1426 | 0.0473 | -0.3988 | 0.3217 | -0.0773 | -0.1359 | -0.2181 | 0.1877 | -0.1200 |
| Ag x | -0.0233 | -0.1119 | -0.1651 | -0.2992 | 0.0148 | -0.2139 | 0.0133 | 0.3262 | 0.0221 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| y | 0.1653 | 0.0582 | 0.2009 | 0.0756 | -0.0811 | -0.2830 | -0.2145 | 0.1534 | -0.0939 |
| z | -0.1018 | 0.1764 | 0.2760 | 0.2257 | 0.3928 | -0.1743 | -0.1012 | 0.1950 | 0.1411 |
| Ag x | -0.2439 | 0.4075 | -0.0254 | -0.1570 | 0.1334 | -0.0182 | -0.1605 | -0.0748 | -0.0083 |
| y | -0.7408 | -0.0893 | 0.0257 | 0.0101 | -0.1076 | -0.0754 | 0.0437 | 0.0213 | -0.0234 |
| z | -0.0875 | 0.0615 | 0.1262 | -0.0422 | -0.0537 | 0.4854 | -0.0903 | -0.0518 | 0.2542 |
| Ag x | 0.0657 | -0.0487 | 0.0938 | 0.1983 | -0.1357 | 0.2170 | 0.4012 | 0.2843 | -0.3740 |
| y | 0.2922 | -0.1200 | -0.2772 | -0.5579 | -0.0889 | 0.0522 | -0.1517 | -0.0147 | 0.0759 |
| z | 0.0727 | 0.0457 | 0.0971 | -0.1016 | -0.0160 | 0.4112 | -0.0770 | -0.0336 | 0.0966 |
| Sn x | 0.0196 | 0.2181 | -0.1823 | 0.0852 | -0.1482 | -0.0556 | 0.0071 | -0.2379 | -0.2603 |
| y | -0.2256 | -0.0867 | -0.3281 | 0.0905 | 0.0890 | 0.2759 | -0.0718 | 0.1318 | -0.0066 |
| z | 0.0373 | -0.2156 | 0.2110 | -0.1480 | 0.0798 | -0.0673 | 0.0780 | 0.0711 | -0.1995 |
| Sn x | -0.1112 | -0.0140 | -0.0975 | -0.1833 | 0.2602 | -0.0457 | -0.0526 | 0.2982 | -0.0230 |
| y | -0.0285 | -0.0124 | -0.0588 | 0.1773 | -0.1328 | 0.2099 | -0.1314 | -0.0969 | -0.1729 |
| z | -0.1498 | -0.0492 | -0.2412 | 0.0068 | -0.0967 | -0.1097 | 0.2534 | -0.1967 | -0.0335 |
| Sn x | 0.1177 | 0.3340 | 0.0464 | 0.0449 | 0.1887 | 0.1896 | -0.0542 | -0.0997 | 0.0483 |
| y | 0.2336 | -0.0833 | -0.1094 | 0.3849 | 0.1422 | -0.0923 | 0.1070 | -0.0617 | 0.1590 |
| z | 0.0696 | 0.2228 | -0.1967 | -0.0160 | -0.1580 | -0.1716 | 0.0747 | 0.0834 | 0.3702 |
| Sn x | -0.0021 | -0.1785 | -0.0362 | 0.0947 | 0.0140 | -0.0776 | -0.2515 | -0.2885 | 0.0860 |
| y | 0.0097 | 0.1270 | 0.3402 | -0.2094 | -0.1345 | -0.0460 | 0.1022 | -0.0591 | -0.0681 |
| z | 0.0022 | -0.3862 | 0.1619 | -0.0715 | 0.1223 | -0.0787 | -0.0492 | 0.0306 | -0.0754 |
| Sn x | 0.0829 | -0.0267 | 0.1916 | -0.0289 | -0.0155 | -0.1676 | 0.1264 | -0.1332 | 0.1332 |
| y | 0.0448 | 0.0132 | 0.1336 | 0.0698 | -0.0405 | -0.0210 | -0.1902 | 0.2233 | 0.1567 |
| z | 0.1128 | 0.1215 | 0.0422 | -0.0901 | -0.0923 | 0.0775 | -0.1184 | 0.0386 | -0.4836 |

16: 67.9 17: 68.8 18: 76.7 19: 94.2 20: 95.5 21: 104.6 22: 106.5 23: 111.9 24: 115.1

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Ag x | -0.2656 | -0.0494 | 0.2163 | -0.1027 | -0.1519 | 0.2538 | 0.0212 | -0.1954 | 0.0478 |
| y | -0.0213 | -0.1485 | -0.2348 | -0.0491 | -0.0705 | 0.3832 | -0.0162 | -0.1853 | 0.1878 |
| z | -0.0853 | -0.3296 | -0.1465 | 0.0793 | 0.0117 | -0.2018 | 0.0053 | -0.0941 | -0.3270 |
| Ag x | 0.0801 | -0.2018 | 0.1511 | -0.2154 | 0.2451 | 0.1212 | 0.4749 | 0.1490 | -0.0569 |
| y | 0.0798 | -0.0320 | 0.0411 | -0.1562 | -0.2110 | 0.2163 | 0.0271 | -0.2308 | 0.1441 |
| z | 0.1844 | -0.1799 | -0.1966 | -0.1811 | -0.3922 | 0.1430 | 0.0878 | 0.2498 | -0.1785 |
| Ag x | -0.3052 | 0.1779 | -0.3181 | -0.0424 | 0.0472 | 0.0953 | 0.1044 | -0.0222 | 0.1895 |
| y | -0.0928 | -0.0570 | -0.0374 | 0.4739 | -0.0148 | 0.0875 | 0.3339 | -0.2143 | -0.1549 |
| z | -0.1466 | -0.1952 | 0.3968 | -0.1441 | -0.1699 | -0.0640 | -0.0726 | 0.0818 | 0.2248 |
| Ag x | 0.0161 | 0.0183 | 0.1446 | -0.2541 | 0.1268 | 0.1160 | -0.0469 | -0.2181 | -0.2970 |
| y | -0.0089 | -0.0061 | 0.0021 | 0.0431 | -0.0339 | -0.0575 | -0.0113 | 0.0873 | 0.1188 |
| z | -0.0472 | 0.0522 | -0.2786 | 0.2801 | -0.1201 | 0.0939 | 0.1499 | -0.0304 | -0.0056 |
| Ag x | -0.0727 | -0.2603 | -0.0347 | 0.1594 | -0.0838 | -0.1183 | -0.3896 | -0.1022 | 0.0712 |
| y | -0.1012 | -0.1392 | 0.3410 | -0.0162 | -0.2181 | -0.1777 | -0.1727 | 0.0967 | 0.0864 |
| z | -0.0564 | -0.0040 | 0.0014 | -0.1456 | 0.0472 | 0.0090 | -0.1580 | -0.1211 | -0.2169 |
| Sn x | 0.0773 | 0.1579 | 0.1746 | 0.0647 | 0.1900 | 0.2544 | -0.0103 | 0.2524 | 0.0538 |
| y | 0.0158 | 0.0614 | 0.1642 | 0.2496 | -0.0568 | 0.1989 | -0.1663 | 0.0037 | -0.2159 |
| z | 0.2318 | 0.3291 | 0.0484 | -0.0873 | -0.1654 | -0.2025 | 0.1618 | -0.1552 | -0.0336 |
| Sn x | 0.1873 | -0.0663 | 0.0098 | 0.0860 | -0.0105 | -0.1784 | 0.1221 | -0.1936 | -0.1682 |
| y | 0.3237 | 0.2135 | 0.0197 | -0.2221 | -0.0291 | -0.2623 | 0.2110 | -0.1578 | 0.2828 |
| z | -0.3878 | 0.1842 | -0.0082 | -0.1101 | -0.1057 | -0.1022 | 0.1162 | 0.0599 | 0.0960 |
| Sn x | -0.2095 | 0.1496 | -0.0785 | 0.2441 | -0.1554 | -0.2355 | 0.1234 | 0.3193 | 0.2162 |
| y | -0.2286 | 0.2797 | 0.1546 | 0.0599 | 0.2604 | -0.2785 | -0.0745 | -0.0590 | -0.2641 |
| z | 0.3168 | 0.0118 | 0.0401 | 0.2232 | 0.3234 | 0.0825 | -0.1237 | -0.1417 | 0.3258 |
| Sn x | 0.2156 | -0.3156 | -0.1671 | 0.0656 | 0.0788 | -0.3227 | -0.1330 | -0.0885 | 0.1983 |
| y | 0.1482 | -0.2163 | 0.0006 | -0.0027 | 0.1017 | -0.0517 | 0.1521 | 0.5036 | -0.1573 |
| z | 0.1283 | 0.1373 | 0.0963 | 0.1813 | 0.1790 | 0.2606 | -0.2345 | 0.2500 | 0.0787 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sn x | 0.2510 | 0.3749 | -0.0906 | -0.0266 | -0.2778 | 0.0360 | -0.2586 | 0.0813 | -0.2568 |
| y | -0.1214 | 0.0266 | -0.4457 | -0.3664 | 0.2466 | -0.0369 | -0.2756 | 0.1349 | -0.0099 |
| z | -0.1451 | -0.0366 | 0.0364 | -0.1009 | 0.3628 | -0.0195 | 0.0683 | -0.0950 | 0.0127 |

25: 116.7 26: 124.5 27: 131.3 28: 137.0 29: 147.6 30: 157.3

| | | | | | | |
|---|---|---|---|---|---|---|
| Ag x | -0.2488 | -0.0894 | -0.1133 | -0.0381 | 0.0006 | 0.0208 |
| y | -0.1226 | -0.1964 | -0.1381 | -0.0492 | 0.0245 | -0.0187 |
| z | -0.3786 | 0.0631 | 0.2745 | 0.2860 | -0.0716 | -0.0238 |
| Ag x | -0.0217 | 0.0471 | -0.0957 | 0.0546 | -0.0132 | 0.0393 |
| y | 0.1433 | 0.5206 | 0.1529 | 0.0127 | 0.0151 | 0.0250 |
| z | 0.0292 | -0.0353 | 0.0125 | 0.0036 | 0.0379 | -0.0122 |
| Ag x | 0.1907 | -0.1880 | 0.1821 | 0.4138 | -0.0671 | -0.1249 |
| y | 0.1390 | 0.0090 | -0.0100 | -0.0746 | 0.1468 | -0.1316 |
| z | 0.0352 | -0.0921 | 0.0757 | 0.1258 | -0.1063 | 0.0402 |
| Ag x | 0.2277 | -0.1353 | 0.1636 | -0.0847 | -0.1091 | 0.0667 |
| y | -0.1036 | 0.0675 | -0.0924 | 0.0547 | 0.0953 | -0.0769 |
| z | 0.0833 | -0.1154 | 0.2384 | -0.1734 | -0.3228 | 0.2967 |
| Ag x | 0.0197 | -0.2653 | 0.0489 | -0.0989 | -0.0497 | -0.0158 |
| y | -0.0679 | -0.0404 | 0.0656 | -0.0769 | -0.0827 | 0.0802 |
| z | 0.1169 | -0.0197 | -0.0619 | 0.1138 | 0.4345 | -0.5588 |
| Sn x | -0.1260 | 0.0771 | 0.2025 | -0.1716 | -0.2332 | -0.2920 |
| y | 0.0597 | 0.1375 | -0.2719 | 0.2374 | -0.1779 | 0.0158 |
| z | -0.0692 | 0.0672 | -0.1968 | -0.0725 | -0.4850 | -0.3319 |
| Sn x | -0.2798 | 0.0859 | 0.0350 | -0.3976 | 0.2781 | 0.1173 |
| y | -0.0700 | -0.2351 | 0.3268 | 0.1721 | 0.2111 | 0.0972 |
| z | 0.2863 | -0.0401 | -0.1802 | -0.4322 | 0.2134 | 0.0864 |
| Sn x | -0.2542 | 0.2258 | -0.1140 | 0.1281 | 0.1358 | -0.0908 |
| y | 0.0777 | -0.0921 | 0.1303 | -0.0052 | -0.0797 | 0.0382 |
| z | -0.1387 | -0.2770 | -0.2776 | -0.0140 | 0.0328 | -0.0274 |
| Sn x | 0.4778 | 0.2841 | -0.0876 | 0.0053 | -0.1124 | -0.0498 |
| y | 0.1936 | -0.2982 | -0.1159 | -0.0196 | -0.0013 | -0.0092 |
| z | 0.0616 | 0.2141 | 0.4157 | -0.0589 | 0.2423 | 0.0838 |
| Sn x | 0.0224 | -0.0715 | -0.2129 | 0.2007 | 0.1590 | 0.3287 |
| y | -0.2498 | 0.1446 | -0.0484 | -0.2577 | -0.1418 | -0.0256 |
| z | -0.0312 | 0.2260 | -0.2750 | 0.2386 | 0.0234 | 0.4350 |