

Vibrational corrections at the CCSD(T)/cc-pVTZ level

| Isotopolog | A_0 | B_0 | C_0 | ΔA_0 | ΔB_0 | ΔC_0 | A_e | B_e | C_e |
|-------------------------------------|-----------|-----------|-----------|--------------|--------------|--------------|------------|----------|----------|
| CH ₃ CCH | 159140.40 | 8545.8700 | | 1984.9418 | 27.3535 | | 161125.342 | 8573.231 | |
| CH ₃ C ¹³ CH | | 8290.2465 | | 1984.5151 | 26.4944 | | | 8316.741 | |
| CH ₃ ¹³ CCH | | 8542.3326 | | 1988.9022 | 27.3740 | | | 8569.707 | |
| ¹³ CH ₃ CCH | | 8313.2489 | | 1976.8318 | 25.7667 | | | 8339.016 | |
| CH ₃ CCD | | 7788.1692 | | 1979.6560 | 20.8302 | | | 7808.999 | |
| CH ₃ C ¹³ CD | | 7592.9160 | | 1979.2629 | 20.3510 | | | 7613.267 | |
| CH ₃ ¹³ CCD | | 7787.0256 | | 1983.5697 | 20.8536 | | | 7807.879 | |
| ¹³ CH ₃ CCD | | 7576.8004 | | 1971.5790 | 19.5635 | | | 7596.364 | |
| CH ₂ DCCH | 121836.9 | 8155.6859 | 8025.4765 | 1267.7008 | 24.7259 | 28.4726 | 123104.601 | 8180.412 | 8053.949 |
| CH ₂ DC ¹³ CH | 121830.7 | 7908.4470 | 7785.9107 | 1266.9306 | 23.9879 | 27.5265 | 123097.631 | 7932.435 | 7813.437 |
| CH ₂ D ¹³ CCH | 121825.1 | 8150.5128 | 8020.4263 | 1269.7140 | 24.7447 | 28.4774 | 123094.814 | 8175.258 | 8048.904 |
| ¹³ CH ₂ DCCH | 121736.7 | 7956.7860 | 7832.3491 | 1259.2978 | 23.3883 | 26.9862 | 122995.998 | 7980.174 | 7859.335 |
| CH ₂ DCCD | | 7440.7645 | 7331.9742 | 1259.8481 | 18.8487 | 22.1190 | | 7459.613 | 7354.093 |
| CHD ₂ CCH | | 7765.7006 | 7630.9493 | 927.4891 | 24.1955 | 27.4342 | | 7789.896 | 7658.383 |
| CD ₃ CCH | | 7355.7657 | | 728.9634 | 25.1973 | | | 7380.963 | |
| CHD ₂ CCD | | 7095.0744 | 6982.5539 | 922.2839 | 18.6269 | 21.4717 | | 7113.701 | 7004.026 |
| CD ₃ CCD | | 6734.3258 | | 725.9928 | 19.7150 | | | 6754.041 | |

Vibrational corrections at the ae-CCSD(T)/cc-pwCVTZ level

| Isotopolog | A_0 | B_0 | C_0 | ΔA_0 | ΔB_0 | ΔC_0 | A_e | B_e | C_e |
|-------------------------------------|-----------|-----------|-----------|--------------|--------------|--------------|------------|----------|----------|
| CH ₃ CCH | 159140.40 | 8545.8700 | | 1999.1134 | 27.2986 | | 161139.513 | 8573.176 | |
| CH ₃ C ¹³ CH | | 8290.2465 | | 1998.6682 | 26.4338 | | | 8316.680 | |
| CH ₃ ¹³ CCH | | 8542.3326 | | 2003.0256 | 27.3180 | | | 8569.651 | |
| ¹³ CH ₃ CCH | | 8313.2489 | | 1990.9303 | 25.7109 | | | 8338.960 | |
| CH ₃ CCD | | 7788.1692 | | 1993.7754 | 20.7959 | | | 7808.965 | |
| CH ₃ C ¹³ CD | | 7592.9160 | | 1993.3637 | 20.3142 | | | 7613.230 | |
| CH ₃ ¹³ CCD | | 7787.0256 | | 1997.6415 | 20.8185 | | | 7807.844 | |
| ¹³ CH ₃ CCD | | 7576.8004 | | 1985.6284 | 19.5283 | | | 7596.329 | |
| CH ₂ DCCH | 121836.9 | 8155.6859 | 8025.4765 | 1277.8229 | 24.6748 | 28.4649 | 123114.723 | 8180.361 | 8053.941 |
| CH ₂ DC ¹³ CH | 121830.7 | 7908.4470 | 7785.9107 | 1277.0469 | 23.9316 | 27.5144 | 123107.747 | 7932.379 | 7813.422 |
| CH ₂ D ¹³ CCH | 121825.1 | 8150.5128 | 8020.4263 | 1279.8069 | 24.6929 | 28.4690 | 123104.907 | 8175.206 | 8048.895 |
| ¹³ CH ₂ DCCH | 121736.7 | 7956.7860 | 7832.3491 | 1269.3374 | 23.3360 | 26.9755 | 123006.037 | 7980.122 | 7859.325 |
| CH ₂ DCCD | | 7440.7645 | 7331.9742 | 1269.8933 | 18.8173 | 22.1235 | | 7459.582 | 7354.098 |
| CHD ₂ CCH | | 7765.7006 | 7630.9493 | 934.9429 | 24.1725 | 27.4465 | | 7789.873 | 7658.396 |
| CD ₃ CCH | | 7355.7657 | | 734.5876 | 25.2162 | | | 7380.982 | |
| CHD ₂ CCD | | 7095.0744 | 6982.5539 | 929.6889 | 18.6189 | 21.4928 | | 7113.693 | 7004.047 |
| CD ₃ CCD | | 6734.3258 | | 731.5833 | 19.7421 | | | 6754.068 | |