

P5409: Predictions of line-shape parameters and their temperature dependences by requantized classical dynamics simulations (rCMDS)

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- rCMDS are used to predict line shape of linear molecules such as CO_2 , N_2O , O_2 , ...
- The simulated spectra are then fit with various line-shape models accounting for the Dicke narrowing, speed dependence and line mixing effects, providing the corresponding line-shape parameters for wide range of J''
- The temperature dependences of line-shape parameters were also deduced
- Comparisons with available experimental values show very good agreement

