503
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Title:Comparison of trajectory models in calculations of N-2-broadened half-widths and N-2-induced line shifts for the rotational band of (H2O)-O-16 and comparison with measurements
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Abstract:In this work, Complex Robert-Bonamy calculations of half-widths and line shifts were done for N-2-broadening of water for 1639 transitions in the rotational band using two models for the trajectories. The first is a model correct to second order in time, the Robert-Bonamy parabolic approximation. The second is the solution of Hamilton's equations. Both models use the isotropic part of the atom-atom potential to determine the trajectories. The present calculations used an intermolecular potential expanded to 20th order to assure the convergence of the half-widths and line shifts. The aim of the study is to assess if the difference in the half-widths and line shifts determined from the two trajectory models is greater than the accuracy requirements of the spectroscopic and remote sensing communities. The results of the calculations are compared with measurements of the half-widths and line shifts. It is shown that the effects of the trajectory model greatly exceed the needs of current remote sensing measurements and that line shape parameters calculated using trajectories determined by solving Hamilton's equations agree better with measurement. 
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