CALCULATING RO-VIBRATIONAL SPECTRA OF VAN DER WAALS MOLECULES

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Van der Waals molecules are loosely bound and strongly coupled and their spectroscopy can therefore not be understood with a rigid rotor + harmonic oscillator model. Useful insight can be obtained by numerically solving the ro-vibrational Schroedinger equation using a basis set. The most obvious impediment is the size of the basis required to obtain converged results. Nonetheless, by using an iterative eigensolver and exploiting the structure of quadrature approximations for potential matrix elements, it is possible to do calculations for many molecules of interest. I shall discuss how the choice of the vibrational coordinates and the molecule-fixed axis system influence the calculation of ro-vibrational spectra of Van der Waals molecules and present new results for $(NNO)_2$, H_2-H_2O, and SF_6-He_2.