



GESELLSCHAFT DEUTSCHER CHEMIKER E.V.
Ortsverband Bielefeld

Chemisches Kolloquium

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Computing spectra of Van der Waals clusters

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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. Using an accurate potential and solving the ro-vibrational Schroedinger equation we have studied (NNO)₂. Numerical results will be presented and advantages of different coordinate systems will be discussed.

GDCh-Ortsverband Bielefeld

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