THE ANALYSIS OF THE ROVIBRATIONAL SPECTRUM OF THE HO_2 COMPLEX

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An efficient algorithm has been developed that can be applied to full dimensional calculations of the rovibrational spectrum of triatom molecules. Performance tests of the algorithm on a massively parallel computer, such as the CRAY T3D, indicate that the algorithm scales almost linearly as the number of processors is increased from 4 to 256 processors. Using this parallel implementation of the algorithm on the CRAY T3D, we have calculated the rovibrational spectrum and wavefunctions of HO_2 using the DMBE IV surface of Pastrana, Quintales, Brandao and Varandas.[a] The performance of the algorithm for high values of the total angular momentum, J, is very good. For example, for J = 15 the algorithm achieves over 10 GFlops performance with 256 processors. With this level of performance, it is feasible to predict the spectrum of HO_2 over a wide range of J values. The calculated spectrum will be compared with experimental results where available and with predictions made with simpler theoretical models.

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a. M. R. Pastrana, L. A. M. Quintales, J. Brandão, and A. J. C. Varandas, J. Phys. Chem. **94**, 8073 (1990).