On the structure of liquid phosphorous tribromide (PBr_3)

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Abstract

We have interpreted the structure factor of liquid PBr_3, as measured by Misawa et al.* on a pulsed neutron source, by means of Reverse Monte Carlo modelling. We have used a method of fixed neighbours constraints which accounts for the flexibility of the molecules. Consistency checks, in terms of reference systems generated by hard sphere Monte Carlo, were carried out. From the RMC models, the partial pair correlation functions, partial structure factors and cosine distribution of intramolecular Br-P-Br angles were calculated. We were also able to describe orientational correlations in PBr_3 by means of angular distributions.

* M. Misawa, T. Fukunaga and K. Suzuki, J. Chem. Phys 92, 5486 (1990)