Seminar

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Thermodynamic properties of molecules in electromagnetic fields

External electric or magnetic fields can hybridize rotational states of individual dipolar molecules and thus create directional states whose field-dependent eigenproperties differ qualitatively from those of a rotor or an oscillator. I'll show how quantum statistical mechanics can be used to evaluate ensemble properties of the hybrid states. For linear molecules, the partition function and the averages that determine the thermodynamic functions can be specified by two reduced variables involving the dipole moment, field strength, rotational constant, and temperature. I'll present a simple approximation due to Pitzer that employs the classical partition function with quantum corrections. This provides explicit analytic formulae which permit thermodynamic properties to be evaluated to good accuracy without computing energy levels or state sums. The approximation also yields a generalization of the venerable Langevin-Debye formula for the polarization of an ensemble of dipolar molecules, one which is valid essentially at all field strengths and temperatures.

Wann? Dienstag, 19.09.2006, 14:00 Uhr

Wo? Universität Stuttgart, NWZ II, Raum 2.136