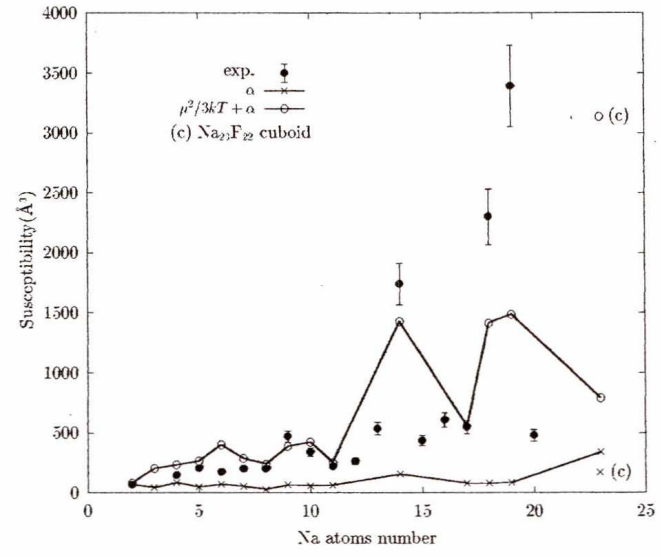
Measurements and calculations of electric dipole moments and polarizabilities of Na_nF_{n-1} clusters

D. Rayane, I. Compagnon, R. Antoine, M. Broyer and Ph. Dugourd, LASIM Lyon
P. Labastie, J.-M. L'Hermite and A. Le Padellec, Laboratoire CAR, IRSAMC Toulouse
F. Spiegelman, F. Calvo and G. Durand, Laboratoire de Physique Quantique, IRSAMC Toulouse
A.R. Allouche, LASIM Lyon

Electric dipole moments of Na_nF_{n-1} clusters have been measured by deflecting a molecular beam in an inhomogeneous electric field. The deflection of a cluster by the electric field is proportional to the time-averaged value of the component of the dipole moment in the electric field direction. For each Na_nF_{n-1} cluster, one can define an electric susceptibility. The experimental values strongly depend on cluster sizes and the largest ones are obtained for clusters with the largest permanent dipole moments (for n= 9, 10, 14, 18, and 19). For a given size the experimental susceptibilities depend on the temperature *T*.

From a theoretical point of view, Na_nF_{n-1} clusters are treated as one electron embedded in the field of n ions Na^+ and of n-1 ions F^-. The quantum treatment of the electron is obtained by means of electron-Na^+ and electron-F^- pseudopotentials. The ions are treated classically by Born- Mayer and coulombic terms. Moreover the polarization of the ionic cores as well as electron-ion correlation are accounted for by means of polarization operators.

We have calculated the permanent dipole moments and the anisotropic polarizabilities of the free clusters. Comparison with experimental results shows that the susceptibilities of the Na_nF_{n-1} clusters are due to the dipole moment $\vec{\mu}$ rather than to the electronic polarizability α. Such a correlation seems to follow a Langevin-type law, and a good interpolation of the experimental results is obtained with $\mu^2 / 3kT + \alpha$. In general, the validity of the Langevin law is based on a boltzmannian model for the fluctuation of the dipole moment. The dipole fluctuations depend on the default type and on the electron localization in the clusters. The theoretical justification that the temperature dependence is of the Langevin type still remains to be fully understood. *



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