



QUANTUM OPTICS SEMINAR

Title: Accurate calculations of permanent and transition dipole moments of dipolar molecules

Speaker: Olivier Dulieu, Laboratoire Aimé-Cotton, cedex, France

Time: Friday, December 2, 2005 at 11:15

Place: 1520-731

Abstract:

The prediction of processes yielding to the formation of ultracold samples of dipolar molecules requires the accurate knowledge of their electronic and spectroscopic properties. Using a standard quantum chemistry approach based on pseudopotentials for atomic core representation, Gaussian basis sets and effective core polarisation potential we investigate the properties of homonuclear and heteronuclear alkali dimers emphasizing on convergence and accuracy issues with respect to the size of the basis sets and to the optimization of effective potentials.

We will first present a first set of results on the permanent dipole moments of the ground and lowest triplet states of all mixed alkali pairs. We will display their variation with the interatomic distance as well with the vibrational level. Most of the results were not previously available elsewhere. A second set of results concerns transition dipole moments for alkali pairs under investigation in various spectroscopic studies, or in cold molecule experiments. Finally, in the perspective of photoassociation of cold francium atoms, we will present preliminary results on potential curves of the francium dimer and of FrRb and FrCs mixed pairs, using a new pseudopotential elaborated in collaboration with F. Spiegelmann in Toulouse (France).

Michael Drewsen