Experimental and theoretical investigations of spectroscopie properties of azobenzene derivatives

Paul Datin, David Carriere, Christophe Fajolles, Jean-Pierre Dognon

Experimental and theoretical investigations of spectroscopic properties of azobenzene derivatives

Paul Datin[1], David Carrière[1], Christophe Fajolles[1], Jean-Pierre Dognon[1]

[1] *NIMBE, CEA, CNRS, Université Paris-Saclay, CEA/Saclay, 91190 Gif-sur-Yvette, France*

A series of azobenzenes was studied using ab initio and DFT methods to determine the substituent effects on the ground and electronically excited states. Azobenzene molecule is known to undergo a photoisomerization from trans to cis conformation upon irradiation by light. The aim of the presentation is twofold. Firstly, we analyze different methods of calculations of electronic excitations of azobenzene molecule by comparing the results with experimental data. Secondly, we present the results of calculations of the UV-Visible spectra of azobenzene derivatives (e.g. Figure 1) and analyze the nature of the experimentally observed excitations.

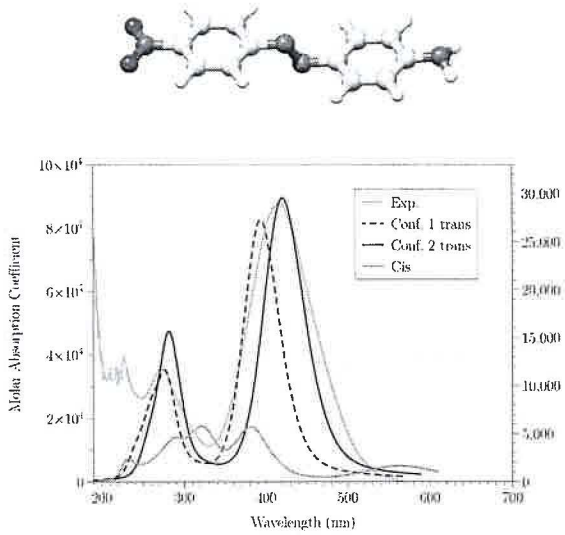

Figure 1: Disperse Orange 3 TD-DFT/CAM-B3LYP vs. experimental UV-Visible spectra