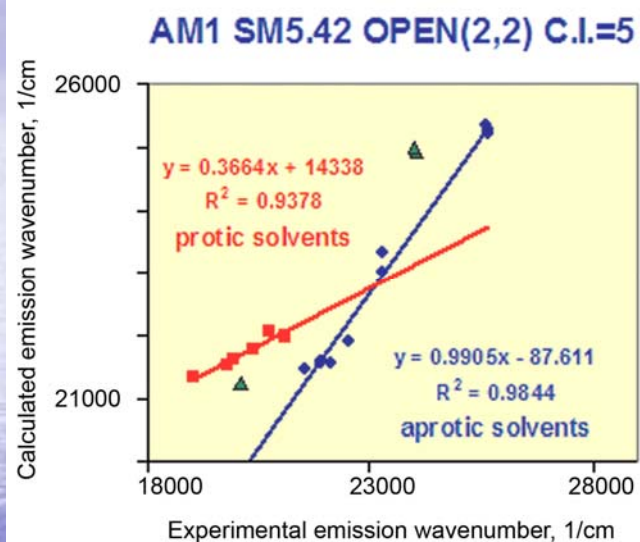
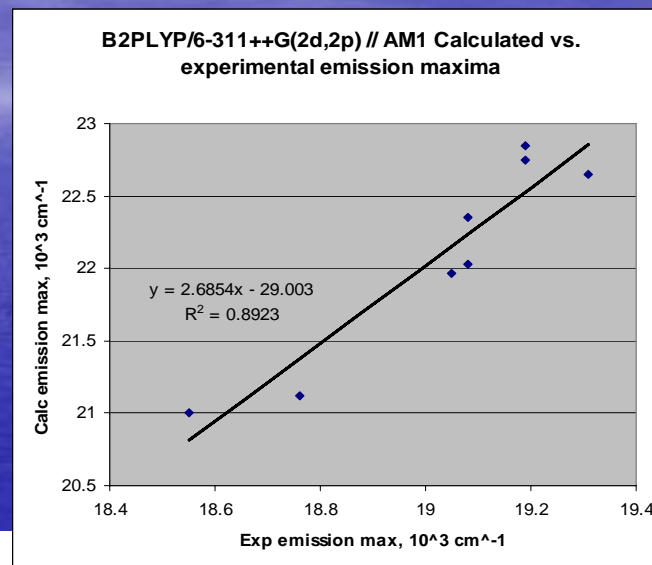
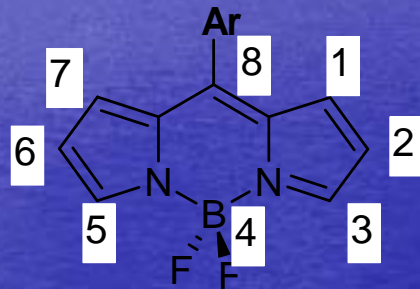


"Reaction Mechanisms and Stereochemistry. Novel Optical Materials" Group

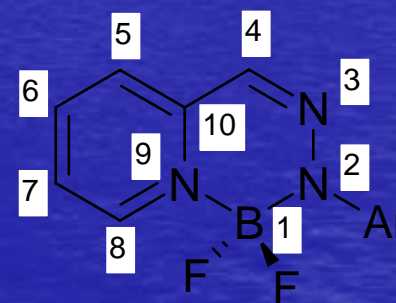
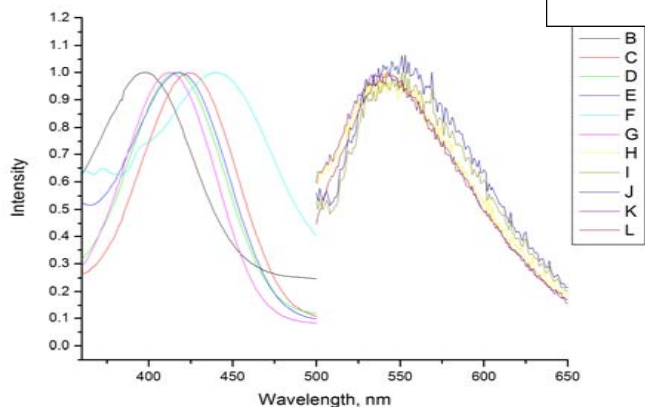
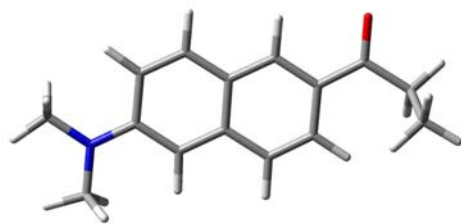
Theoretical Studies and Design of Novel Fluorescent and NLO Materials



Molecules possessing N-B-N fragment(s)



B2PLYP 6-311++G(2d,2p)//CISD AM1



Bakalova, Kaneti, *et al. Bulg. Chem. Commun.*, **2008**, 40, 450-455;
Spectrochim. Acta A **2009**, 72, 36-40;
Chem. Phys. Lett. **2009**, 478, 206-210 – TD DFT and SAC CI computations.

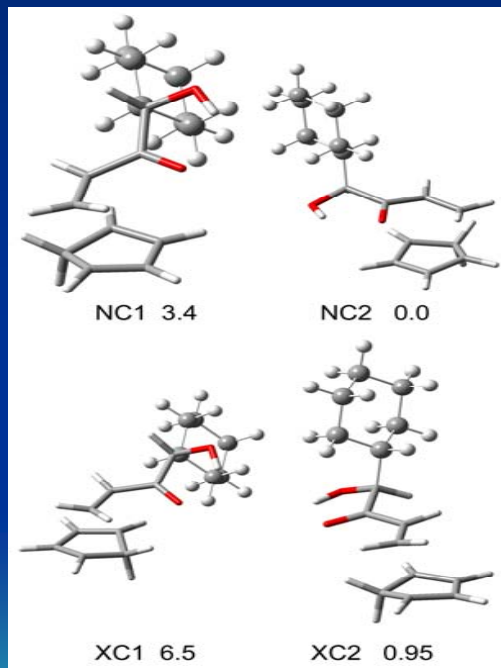
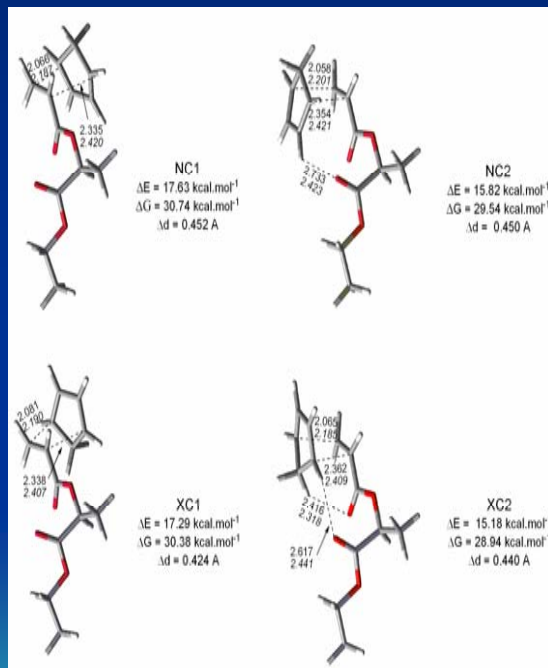
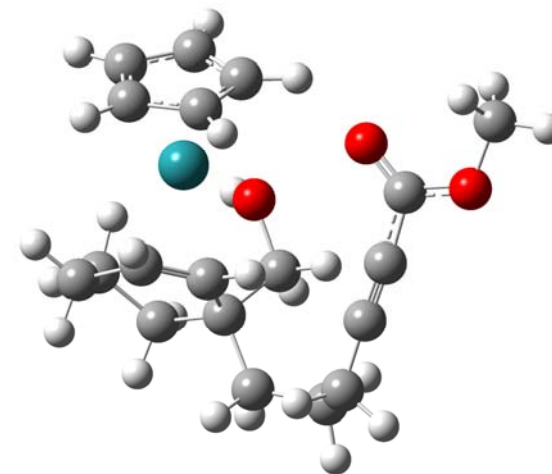
Calc. $\lambda_{\text{max}}^{\text{abs}} = 411 \text{ nm}$
 Exp. 412 nm, CH_3CN
 "Inverse" solvatochromic effect

Mechanism and Stereochemistry

Diels - Alder Additions:

Two types of selectivity – endo/exo, and diastereofacial

Methods – DFT, WFT with explicit electron correlation – MP2 & ONIOM(CCSD : HF)



Cycloisomerization and ene- or enyne rearrangements and additions, e. g. Alder-ene. Catalysis by 4 – 6 row transition metals (from Mn to Au)

Bakalova, Santos: *J. Org. Chem.* **2004**, *69*, 8475;
Eur. J. Org. Chem. **2006**, 1779

Bakalova, Kaneti: *J. Phys. Chem. A*, **2008**, *12(50)*, 13006