How does the solvent affect the absorption and emmission spectra of different type of paints?

Rediet Tegegne

American International School of Budapest
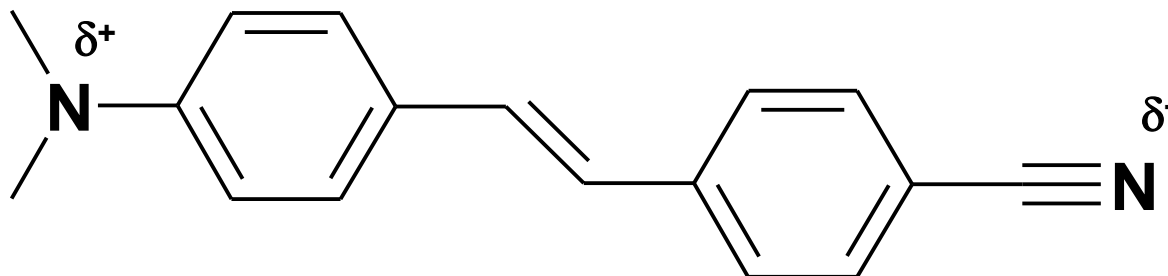*16rtegegne@student.aisb.hu*

"The motto of the mongoose family, so Mr Kipling tells us, is: 'Go and find out."

AKI Kíváncsi Kémikus Miniszimpózium, 2015. július 3.

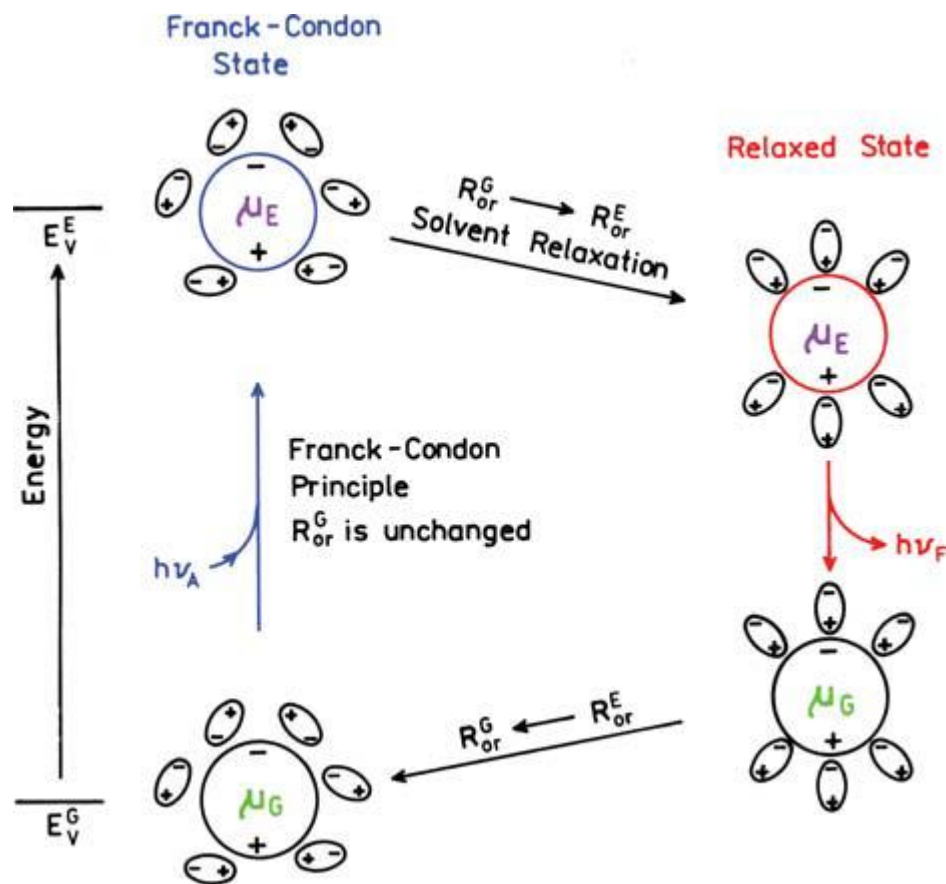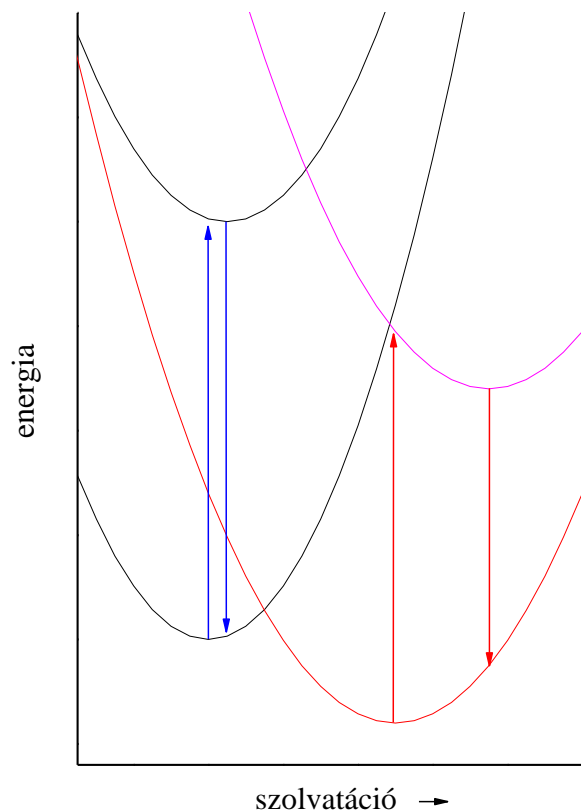# Luminescence of DCS in different solvents

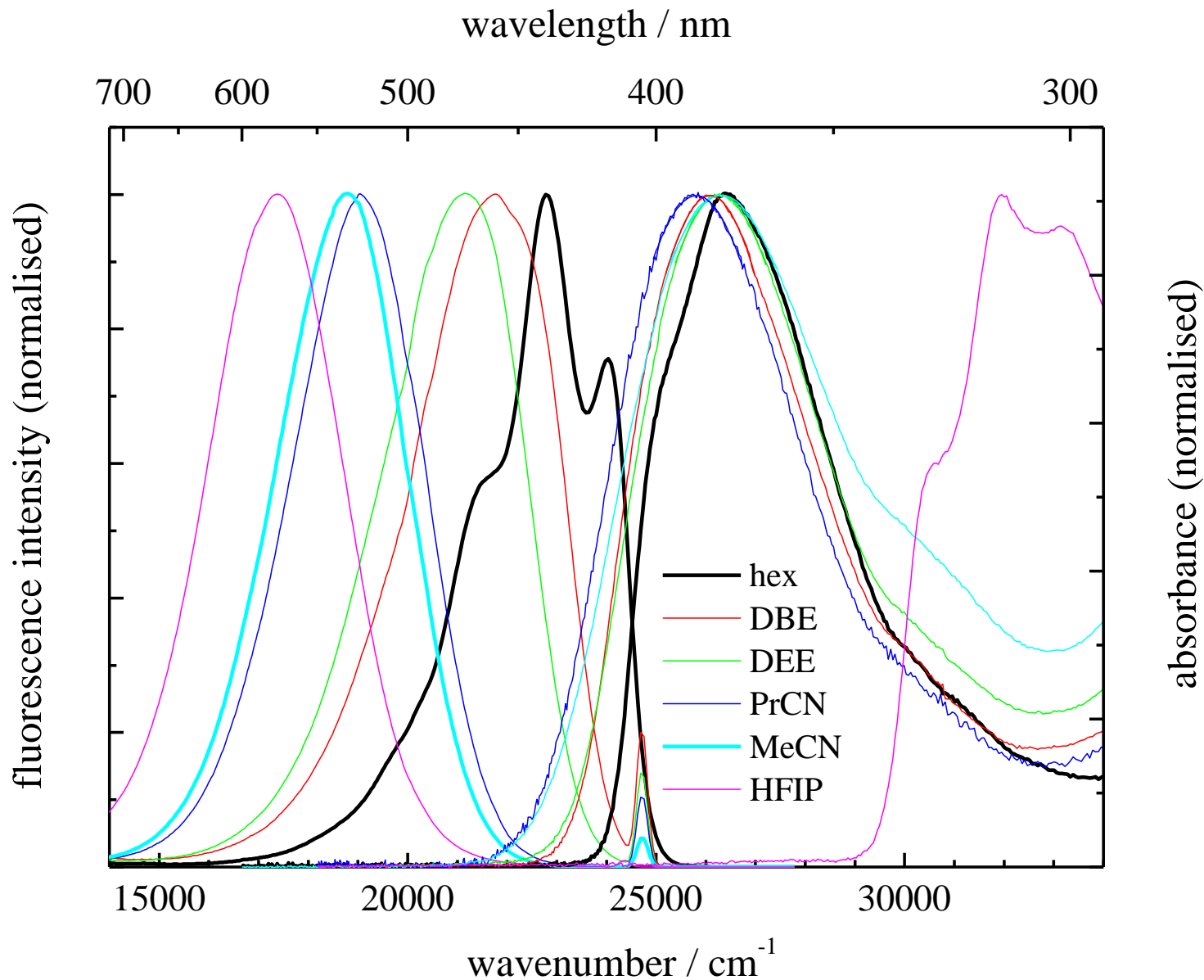**n-hexane**　　　　**acetonitrile**　　　　**hexafluoro-2-propanol**
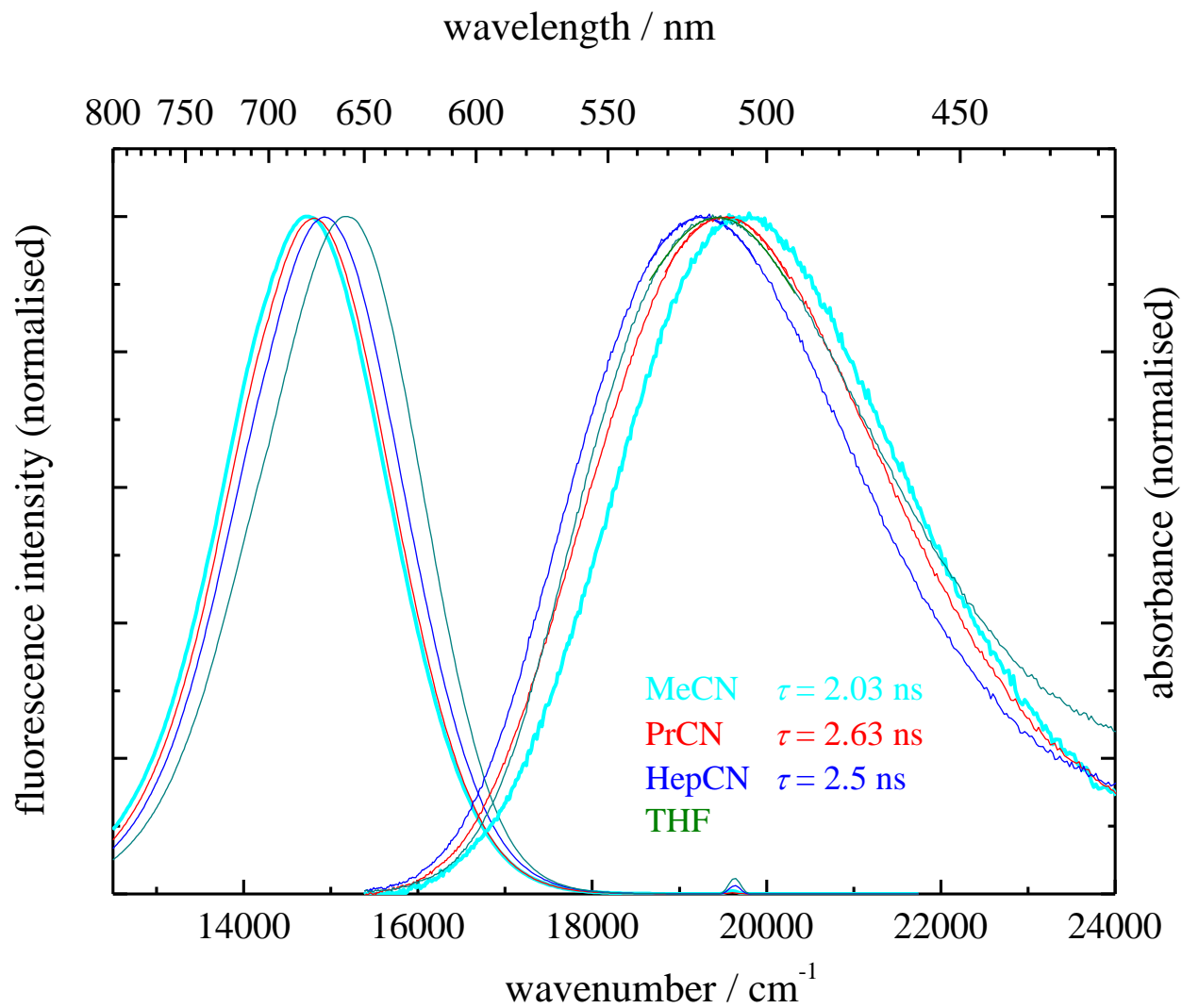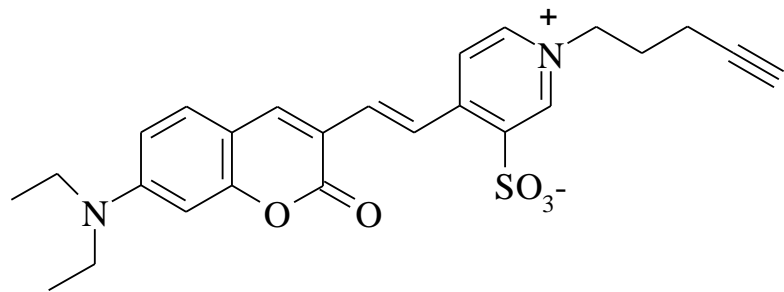
What is a dipole moment (μ)?

The dipole moment is a simplified measure of the polarity of the molecule, the separation of the average positive and negative charges in a species.

{1 electron and 1 proton at 1 angstrom (2 electron and 2 proton at 0.5 angstrom e.t.c.) show **4.8 Debye** dipole moment from far distances}

DCS in different solvents

wavelength / nm

800 750 700 650 600 550 500 450

fluorescence intensity (normalised)

absorbance (normalised)

MeCN $\tau = 2.03$ ns
PrCN $\tau = 2.63$ ns
HepCN $\tau = 2.5$ ns
THF

14000 16000 18000 20000 22000 24000

wavenumber / cm^{-1}

Simplified equations from literature for solvatochromic calculations

Absorption

$$\nu_a{}^{max} = \text{-2 } const. \; \mu_g \, (\mu_e\text{-}\mu_g) \, / \, \rho^3 * (f - f')$$

Fluorescence

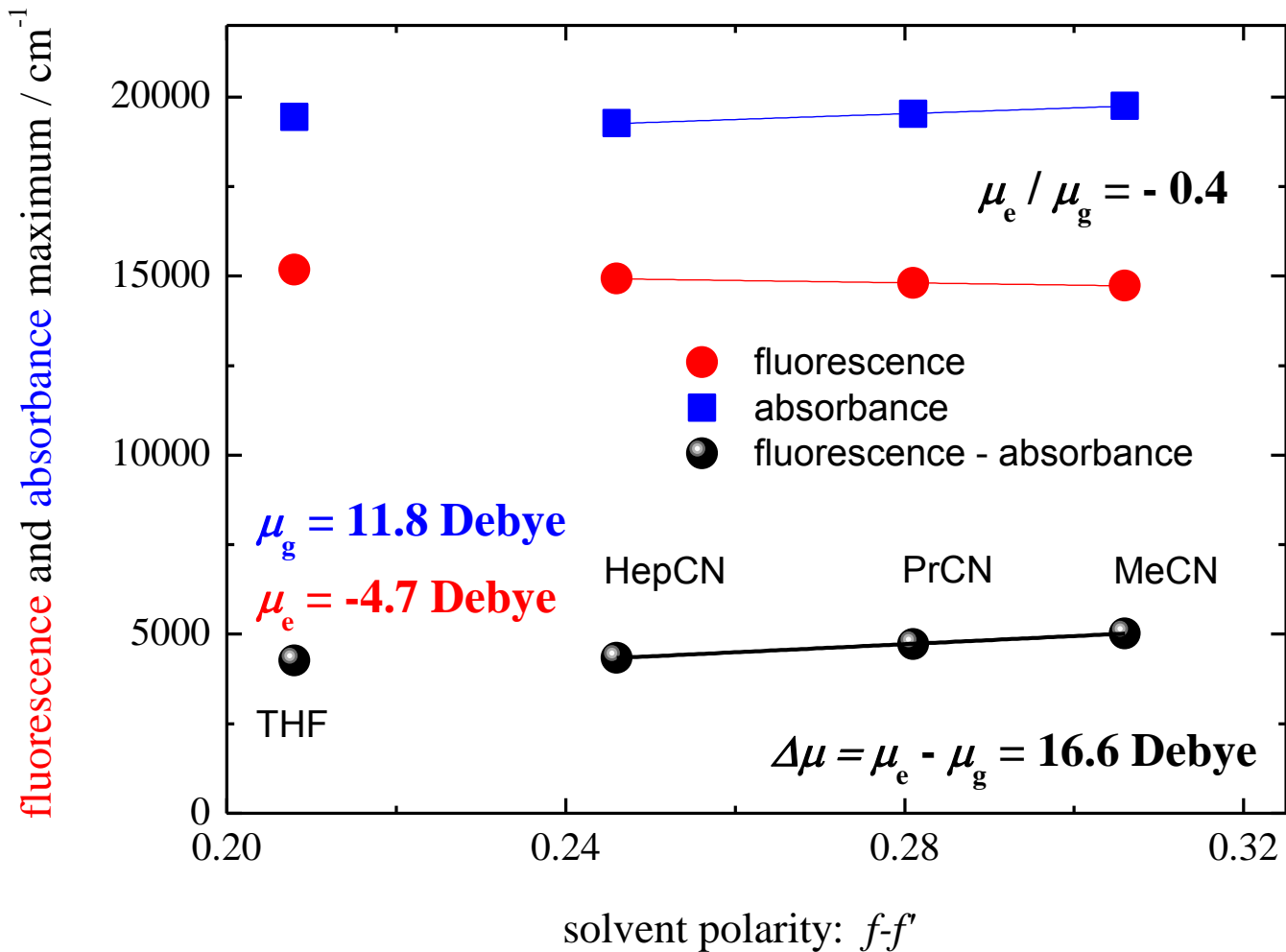$$\nu_f{}^{max} = \text{-2 } const. \; \mu_e \, (\mu_e\text{-}\mu_g) \, / \, \rho^3 * (f - f')$$
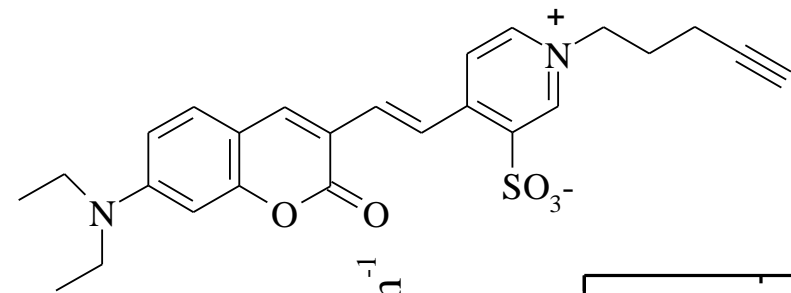
where
$$f - f' = \left(\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}\right)$$

$$\nu_{abs} - \nu_f = \frac{1}{2\pi\varepsilon_0 hc\rho^3}(\mu_e - \mu_g)^2(f - f') + C$$

Solvatochromism of DCS
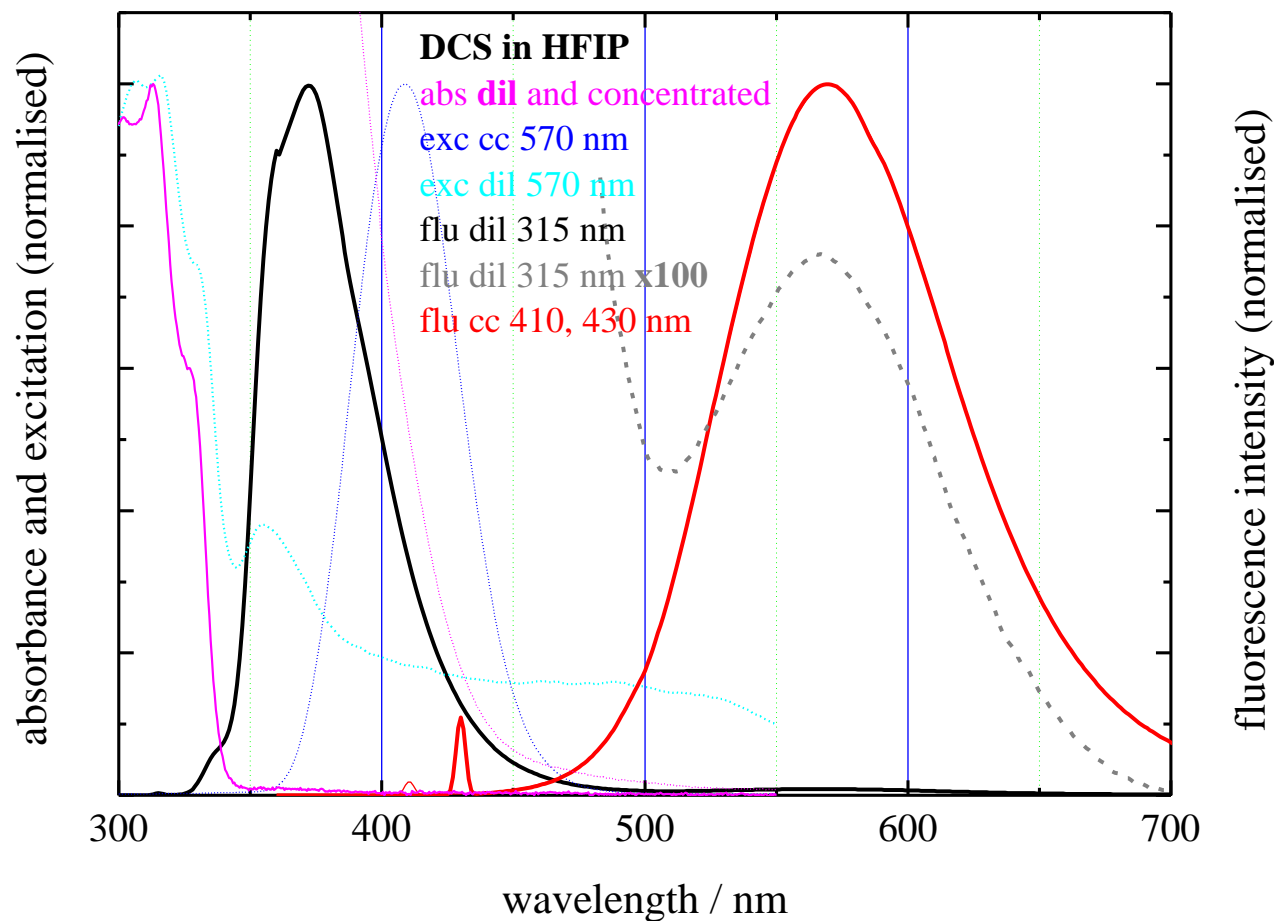

absorption maximum
fluorescence maximum
difference

$\mu_e / \mu_g = 8$

$\mu_g = 2$ Debye *(6 Debye)*

$\mu_e = 16$ Debye *(20 Debye)*

$\mu_e - \mu_g = 14$ Debye

(relativ to DMABN 17)

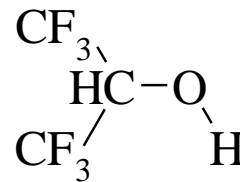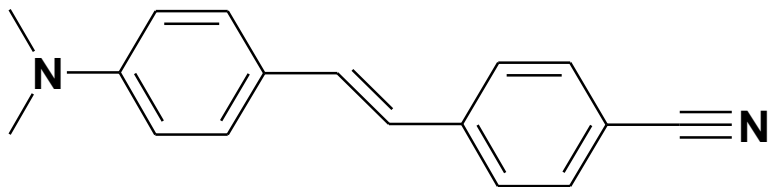fluorescence and absorbance maximum / cm^{-1}

solvent polarity: *f-f'*
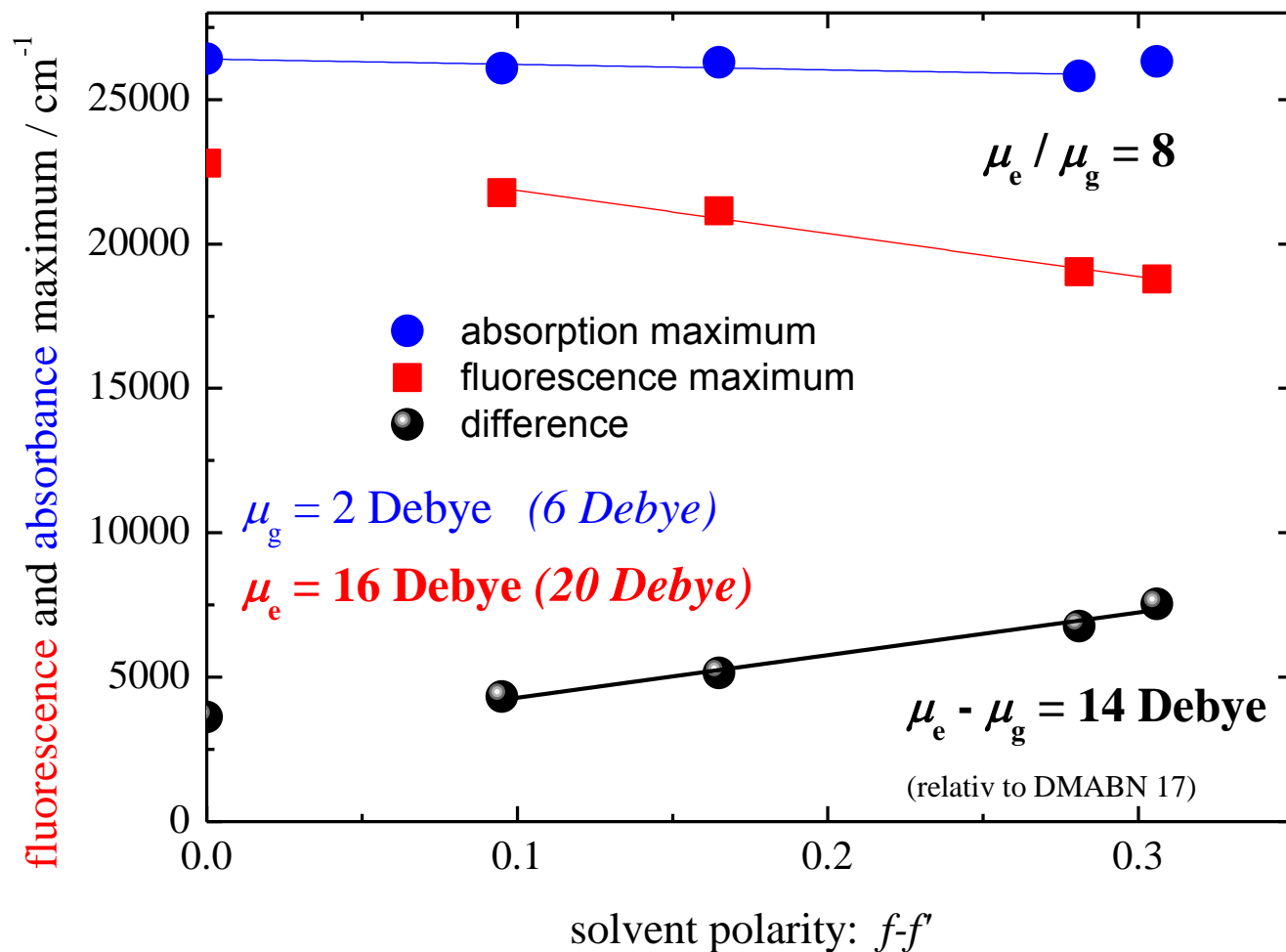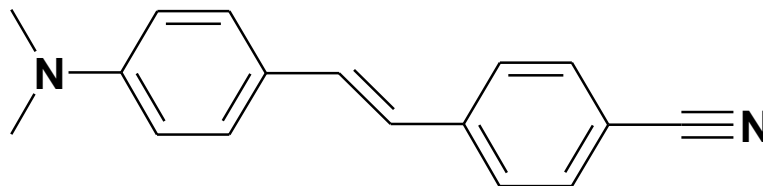
Solvatochromic plot of the red dye

Strange DCS emission in HFIP

Summary:

- The dipole moment of DCS dye is increasing with excitation

- In case of koumarin derivative, the excited states dipole moment is lower than that of ground state, and even the direction of it differs

- The strong hydrogen bonding on the solvent changes the fluorescent properties of DCS in a surprising manner

- The answer to the research question is that the spectra is affected by the polarity of the solvent and the dipole moments of the molecule in ground and excited states as well.

Thank you for this summer program opportunity to the MTA TTK institute, and special thanks to **„Gabi néni"** for all the help, and **Demeter Attila!**

… and thanks for your attention!