Spectral properties of bromocresol purple

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Motivation

- ✓ The pH detector
- ✓ The determination of 2,4,6-trichlorophenol by using a poly(bromocresol purple)/electrochemically reduced graphene oxide composite film
- ✓ The determination of enoxacin by spectrophotometric methods were
- ✓ The determination of oxomemazine hydrochloride in bulk and pharmaceutical formulations by spectrophotometric methods

The goal is to search for characteristics of bromocresol purple to create a sensitive spectroscopic detector

Subject

Bromocresol purple – an organic compound with the chemical formula $C_{21}H_{16}Br_2O_5S$. The structural formula of this dye molecule is shown in Fig. 1.

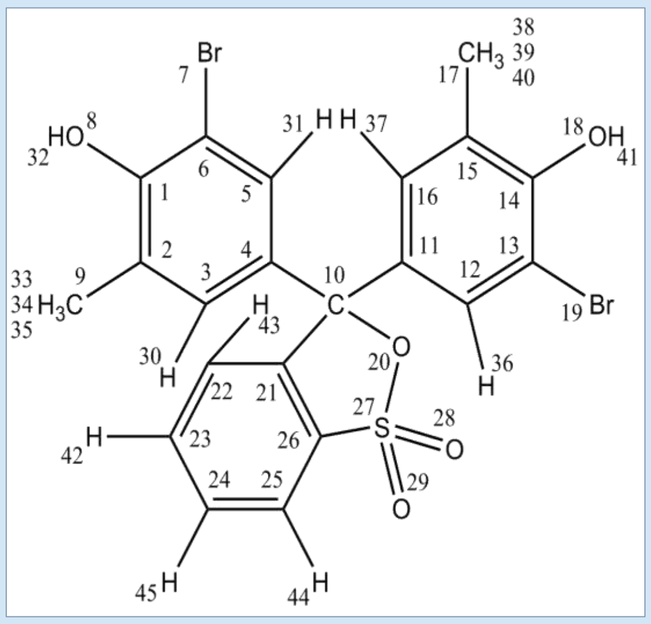

Figure 1. The structural formula of BCP

Solvents

Distilled water (H_2O); ethanol (C_2H_5OH); toluene ($C_6H_5CH_3$); acetone (CH_3COCH_3). Table 1 shows properties.

Table 1. Solvent properties

Solvent	*n*	ε	μ, Д	Donor number	Acceptor number
Water	1.3330	78.5	1.8	18.0	54.8
Ethanol	1.3614	24.3	1.7	19.6	37.9
Acetone	1.3587	20.9	2.8	17.0	12.5
Toluene	1.4969	2.4	0.37	3.6	14

Methods

- Electronic absorption spectroscopy and fluorescence.
- Lippert-Mataga equation:

$$\nu_a - \nu_f \approx \frac{2}{hc}\left(\frac{\varepsilon - 1}{2\cdot\varepsilon + 1} - \frac{n^2 - 1}{2\cdot n^2 + 1}\right)\frac{(\mu^* - \mu)^2}{a^3} + \text{const},$$

From the equation can be expressed the orientational polarizability Δf and dipole moment change $\Delta\mu$:

$$\Delta f = \frac{\varepsilon - 1}{2\cdot\varepsilon + 1} - \frac{n^2 - 1}{2\cdot n^2 + 1},$$

$$\Delta\mu = (\mu^* - \mu) = \sqrt{\frac{mhca^3}{2}},$$

Results

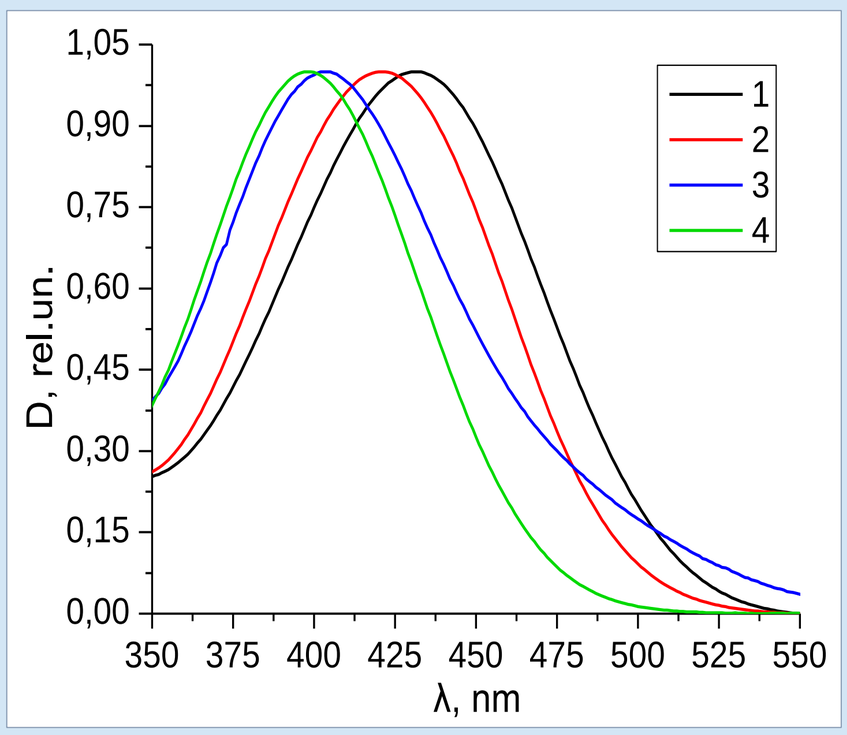

Figure 2. Normalized absorption spectra of BCP:
1 – water; 2 – ethanol; 3 – toluene; 4 – acetone

Table 2. Characteristics of BCP in different solvents

Solvent	λ_{max}, nm	ν_{max}, cm^{-1}	$\Delta\nu_{1/2}$, cm^{-1}	ε, $cm^{-1} \times M^{-1}$	*f*	$\tau\times10^{-9}$, s	λ_{fl}, nm (ν_{fl}, cm^{-1})	ν_{st}, cm^{-1}
Water	433	23100	3600	12600	0.83	0.8	542 (18500)	4600
Ethanol	420	23800	5300	14600	0.36	1.7	543 (18600)	5300
Acetone	398	25200	5000	17500	0.41	1.4	500 (20000)	5200
Toluene	405	24700	6200	500	0.02	42.2	467 (21400)	3300

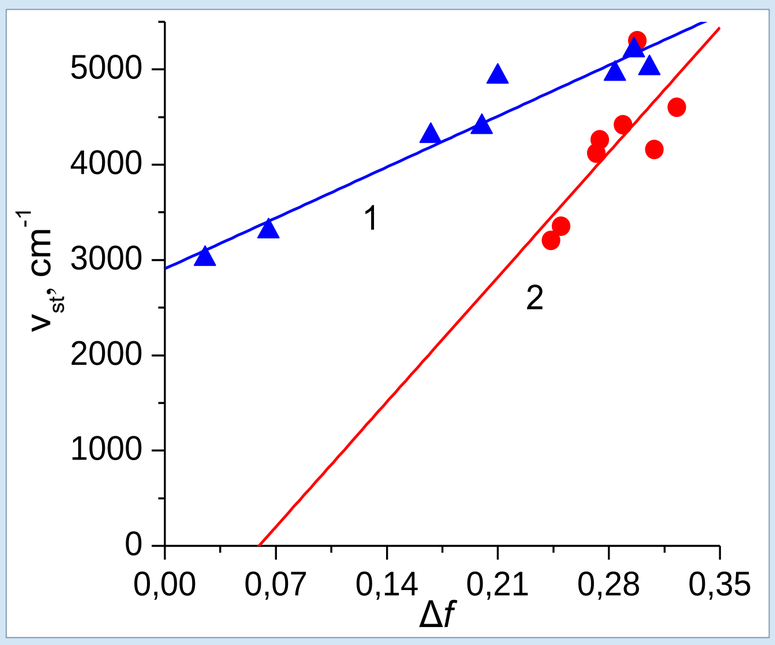

Figure 3. The Lippert-Mataga plots:
1 - protonic; 2 – aprotonic [1]

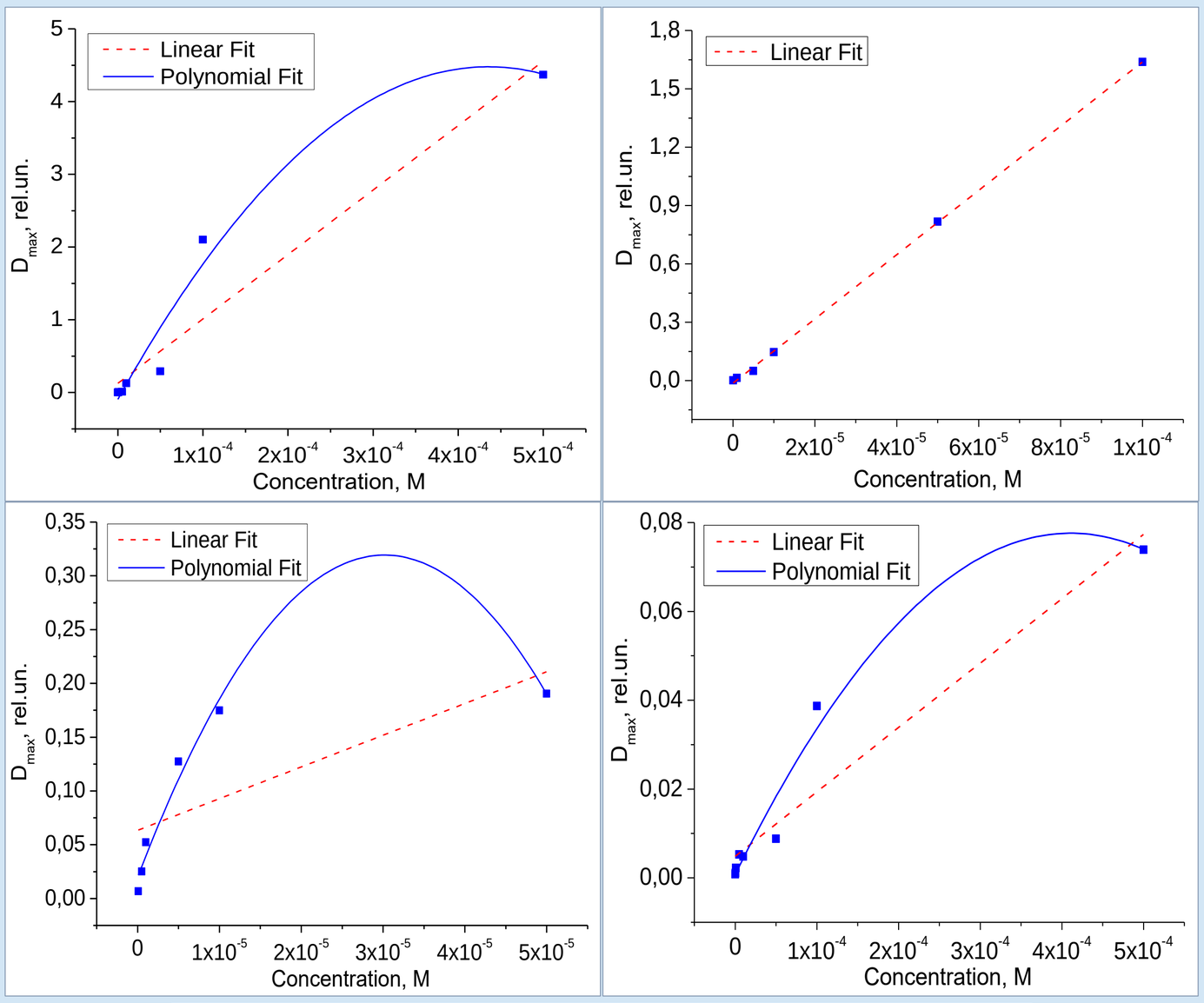

Figure 4. Bouguer-Lambert-Beer low: water (a), ethanol (b), acetone (c) and toluene (d)

Conclusion

1. The change in the dipole moment of BCP upon excitation in protonic solvents (16.2 D) is higher than in aprotic solvents (10.4 D). This is due to the fact that BCP is able to hydrogen bond with protic solvents as both a H-bond donor and a H-bond acceptor. [2]
2. The absorption wavelength in the 350-480 nm spectral region is sensitive to solvent polarity.

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References

1. Talone C. J., Gao J., Lynch J. R., et al. // Spectrochim Acta A. – 2016. – V. 156. – P. 138–142.
2. Bezlepkina N.P., Tchaikovskaya O.N., Bocharnikova E.N. // Izvestiya vuzov. Fizika. – 2022 – № 7.*

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