

# Spectral Response of a Styryl Dye Confined in 1:2 Cucurbit[7]uril Inclusion Complexes

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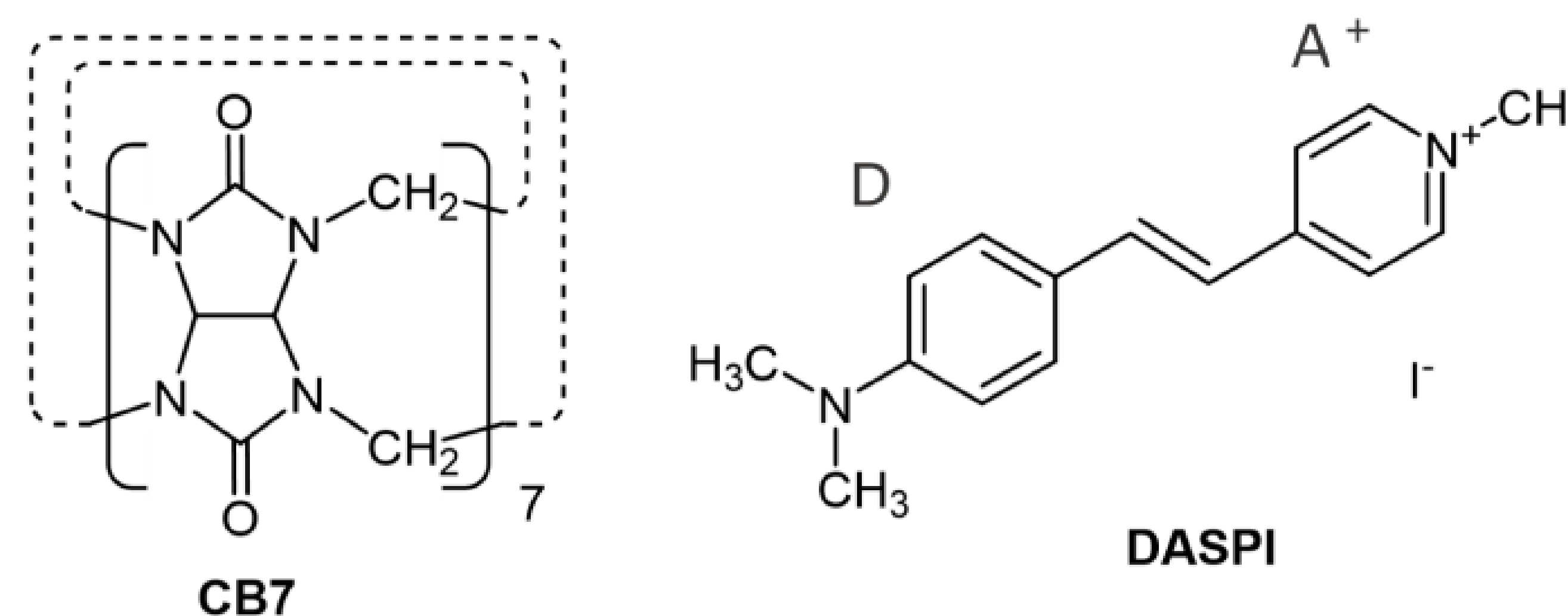
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## INTRODUCTION & AIM

The formation of 1:2 inclusion complexes between the styryl dye DASPI and cucurbit[7]uril (CB[7]) in aqueous solution leads to changes in the absorption and fluorescence spectra of the dye. While similar spectral effects were previously attributed to protonation processes [1], direct pH measurements demonstrate that the addition of CB[7] does not alter acidity under the conditions used [2]. Instead, the observed spectral transformations arise from the specific geometry of triple complexes [3]. Key spectroscopic evidence is provided by a comparative analysis with the isolated donor fragment of DASPI.

## METHOD

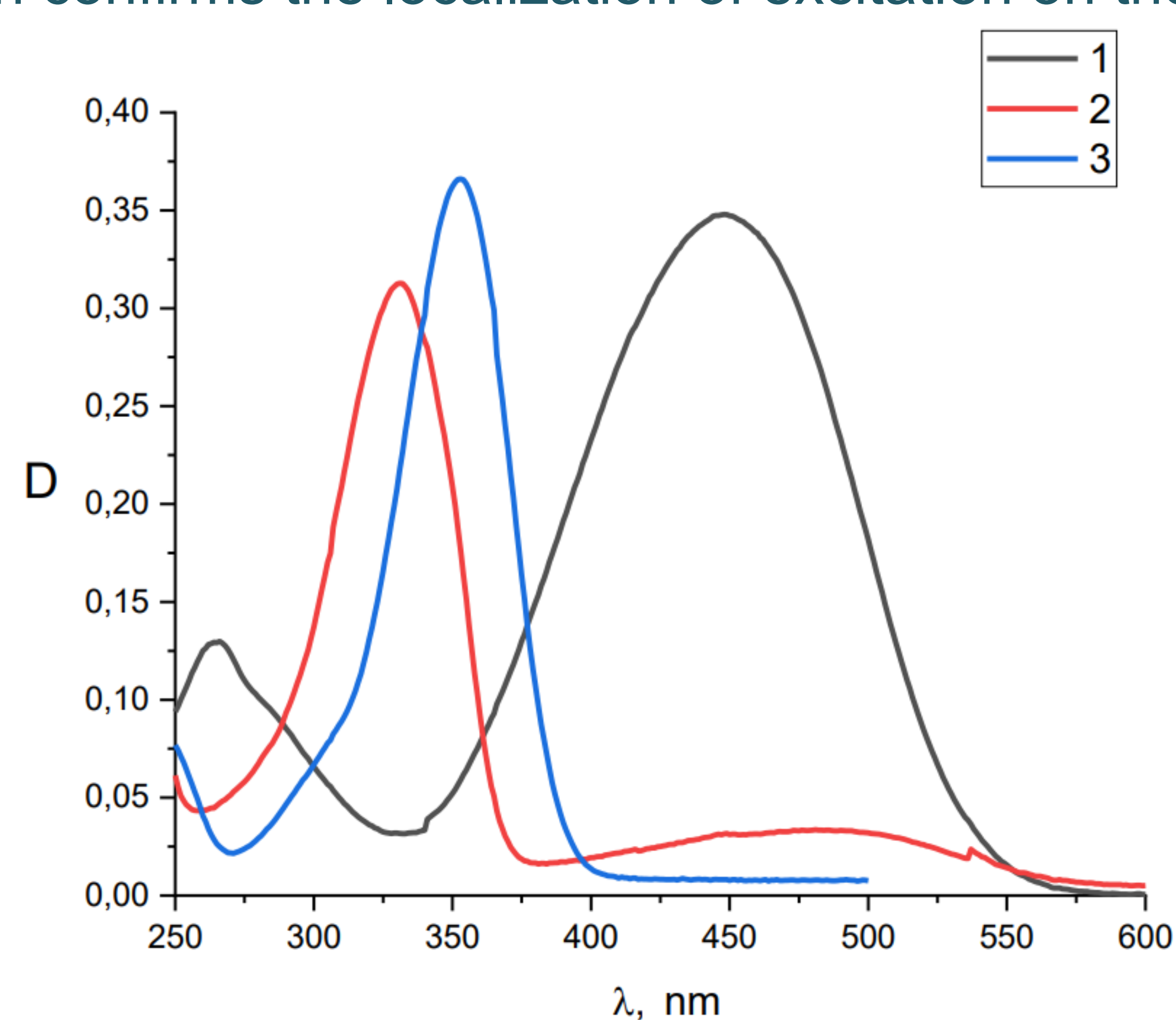
Aqueous solutions of DASPI ( $C = 10^{-5}M$ ) were studied in the free form, in the presence of CB[7], and under acidic conditions, while the donor fragment was investigated separately to establish a reference spectrum. Absorption spectra were recorded using a Shimadzu UVmini-1240.



Structural formulas: CB7 - cucurbit[7]uril, DASPI, D - donor fragment of DASPI, A<sup>+</sup> - acceptor fragment of DASPI.

## RESULTS & DISCUSSION

In the 1:2 complex, two negatively charged portals of CB[7] are located on opposite sides of the  $\pi$ conjugated bridge of DASPI. This arrangement creates an electrostatic field that disrupts the intramolecular charge transfer between donor and acceptor fragments of the dye. As a result, the characteristic long-wavelength band at 450 nm, associated with charge transfer, disappears, and a new band emerges at 330 nm. This new band coincides with the absorption of the isolated donor fragment, which confirms the localization of excitation on the donor part.



Absorption spectra of aqueous solutions of  $10^{-5} M$  DASPI: 1) free, 2) in the presence of 3 eq. CB[7], 3) of the donor fragment

## CONCLUSIONS

Thus, the use of the donor fragment as a spectroscopic reference allowed us to directly demonstrate the mechanism of electrostatic control. The results suggest that tuning the stoichiometry of complexes with cucurbiturils may provide a powerful approach for regulating the optical properties of organic dyes, and can be potentially extended to other supramolecular platforms or sensing applications

## REFERENCES

1. Manna A., Chakravorti S. Spectrochim. Acta A: Mol. Biomol. Spectrosc., 2015, 140, 241–247.
2. Ivanov D.A., Kolesnikova O.P., Kryukov I.V., Petrov N.Kh. High Energy Chem., 2025, 59(3), 222-226.
3. Kolesnikova, O.P.; Ivanov, D.A.; Kryukov, I.V.; Petrov, N.Kh. Chem. Proc., 2025, 18, 120