

SUPPLEMENTARY INFORMATION

Phase Transition Thermochemistry Based on C-H Acidity of 4-Alkylflavylium Compounds in Pluronic® F-127

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1. Crystal packing of the flavylim salt **5b** and the C–H···O hydrogen bonds

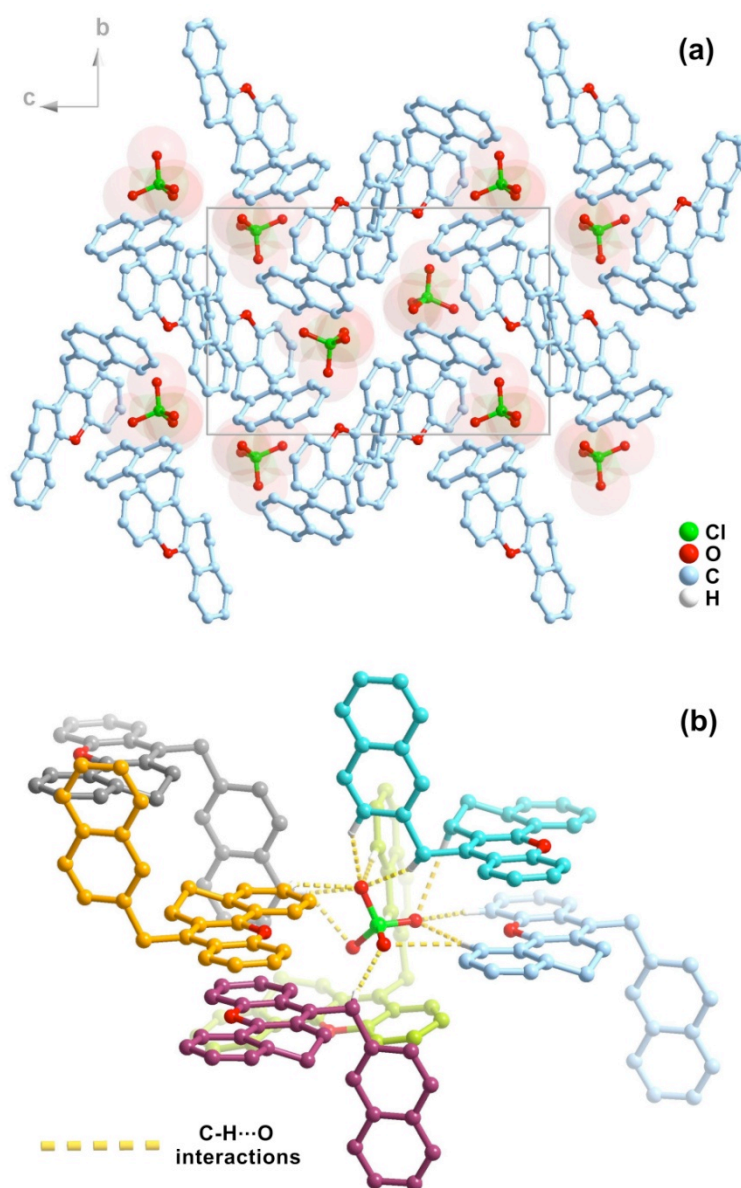


Fig. S1 – a) Crystalline packing arrangement of the compound **5b** viewed in the [1 0 0] direction of the unit cell. b) Weak C–H···O hydrogen bond interactions (shown as golden dashed lines) between the perchlorate anion and the neighboring flavylum molecules; for clarity purpose the carbon atoms of distinct organic molecules are drawn in different colors.

2. UV-Vis spectra of ethylenic bases

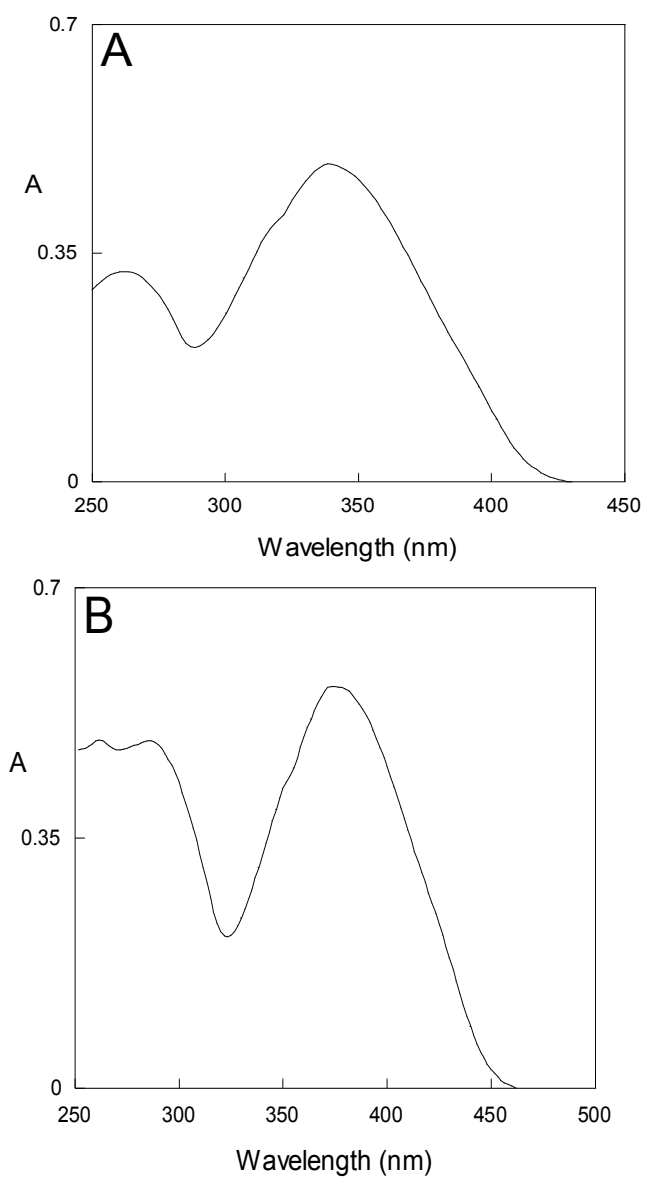


Fig. S2 – UV-Vis spectra of ethylenic base solutions in chloroform:
A. $[6a]=1.3\times 10^{-5}$ M; B. $[6b]=2.0\times 10^{-5}$ M

3. ^1H NMR spectra of 5a and 5b in CDCl_3 and in $\text{D}_2\text{O}/\text{CD}_3\text{OD}$ (1:1) at $\text{pH}\approx 4$, and of 6b in CDCl_3 .

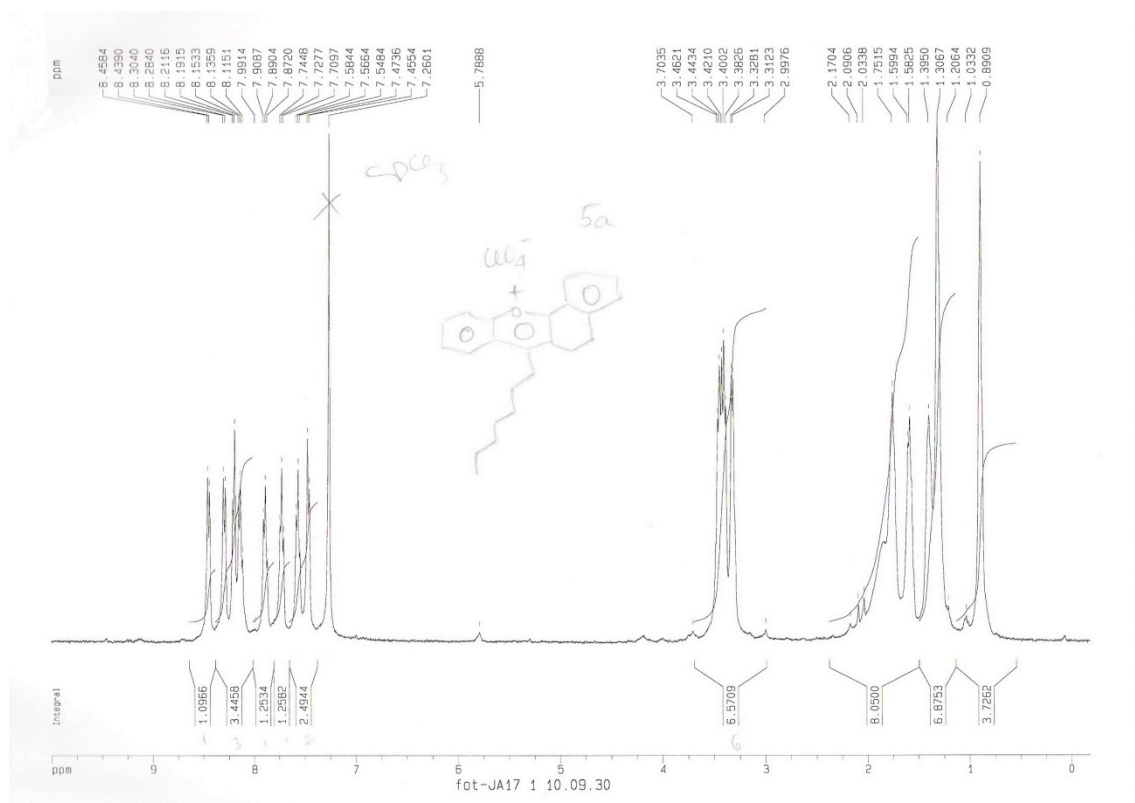


Fig. S3 – ^1H NMR spectrum of 5a in CDCl_3 .

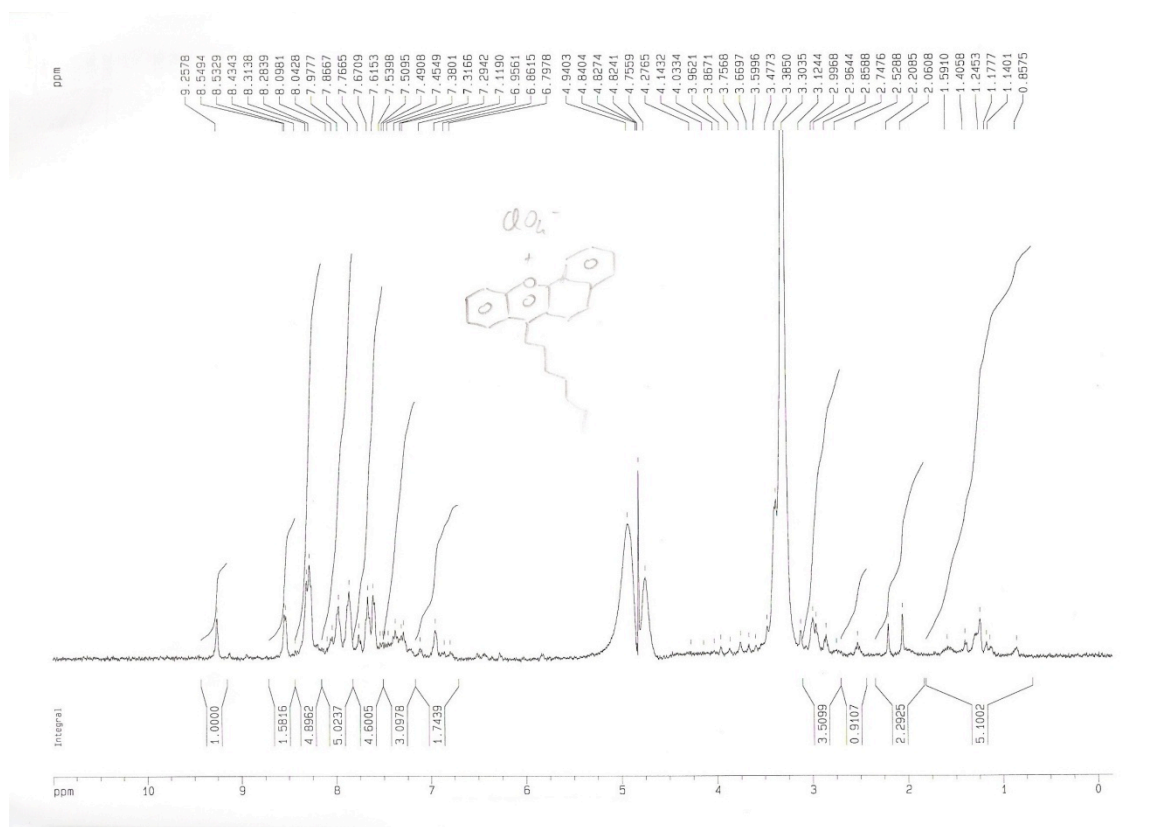


Fig. S4 – ^1H NMR spectrum of 5a in $\text{D}_2\text{O}/\text{CD}_3\text{OD}$ (1:1) at $\text{pH}\approx 4$.

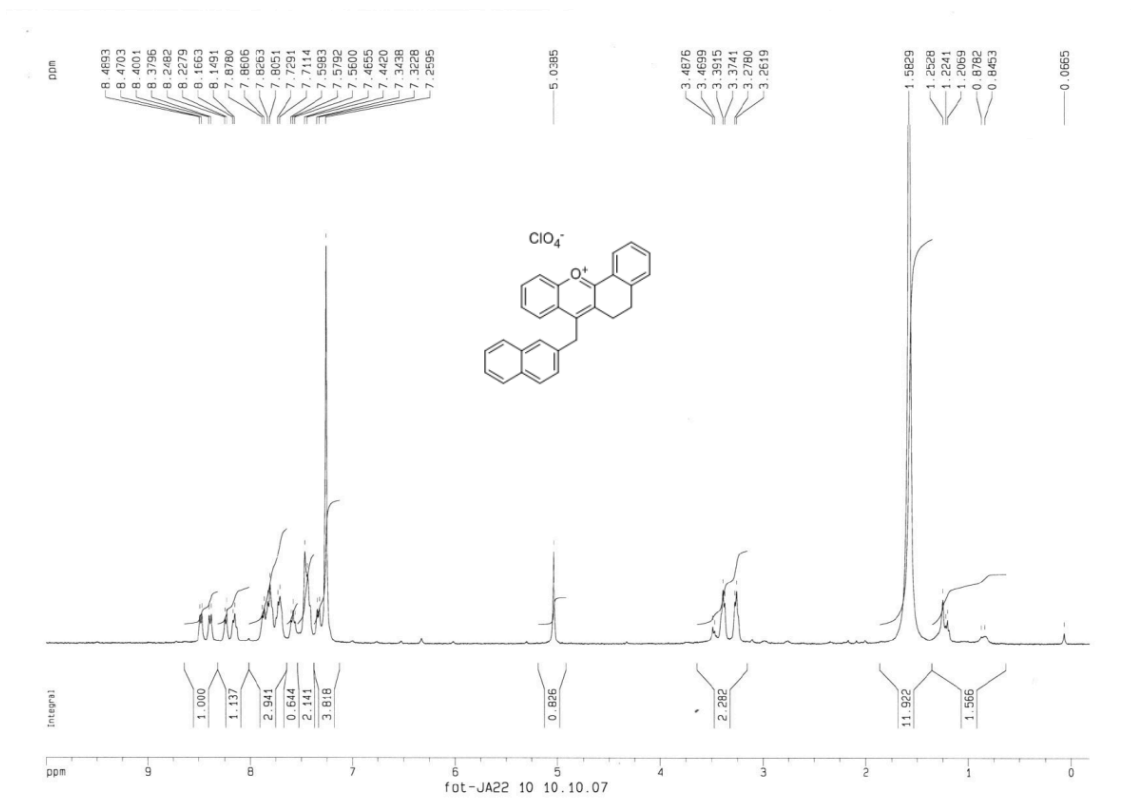


Fig. S5 – ^1H NMR spectrum of **5b** in CDCl_3 .

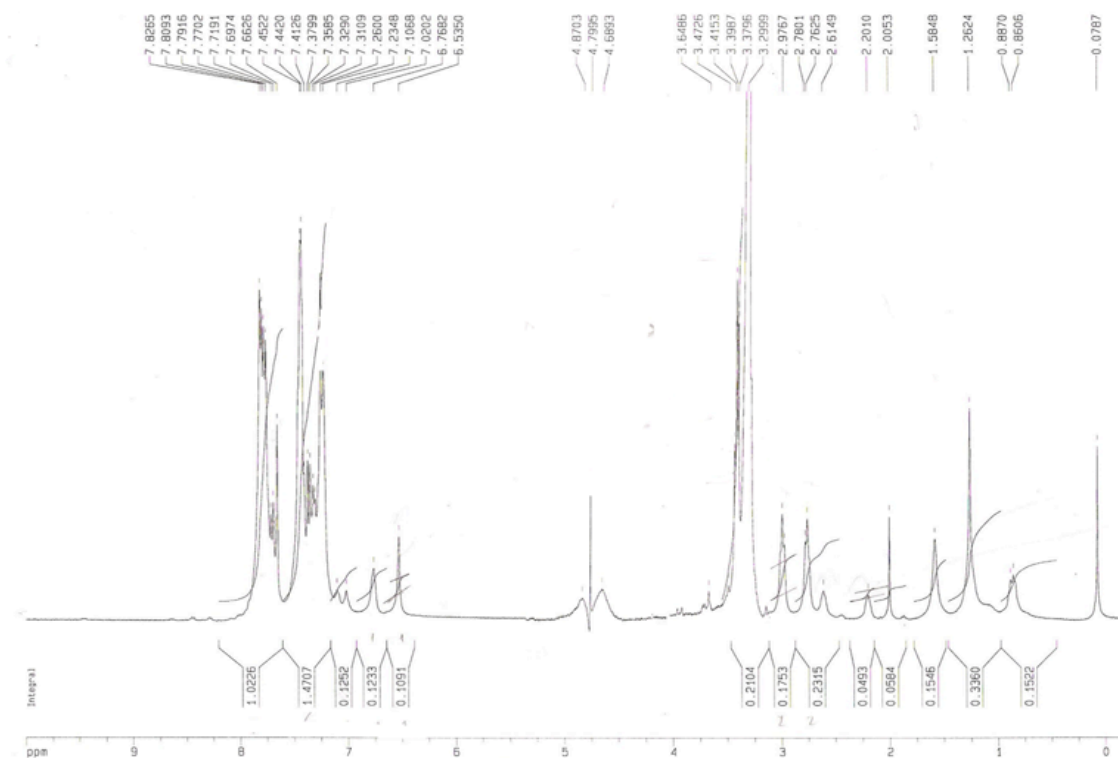


Fig. S6 – ^1H NMR spectrum of **5b** in $\text{D}_2\text{O}/\text{CD}_3\text{OD}$ (1:1) at $\text{pH} \approx 4$.

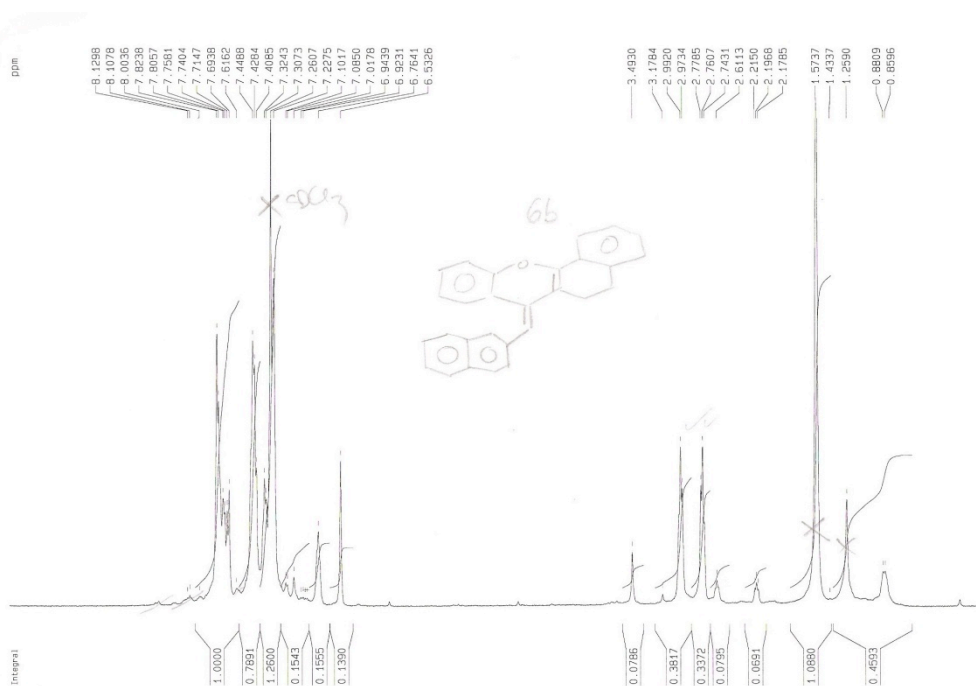


Fig. S7 – ^1H NMR spectrum of **6b** in CDCl_3 .

4. Titration of compounds **1** and **5a** in aqueous 20% (w/v) Pluronic® F127

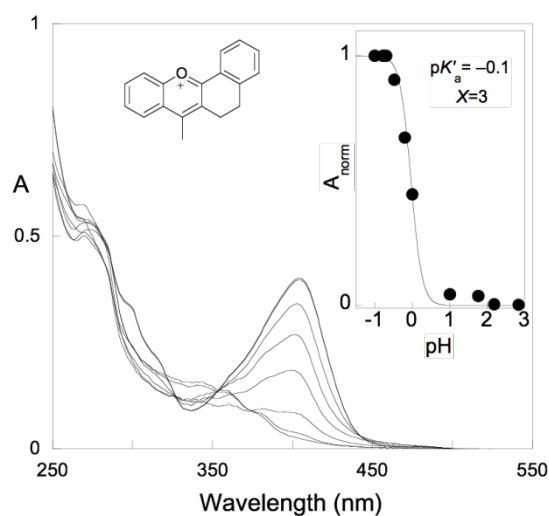


Fig. S8 – Absorption spectra of compound **1** 1.2×10^{-4} M in the presence of 20% (w/v) Pluronic® micelles at room temperature. Fitting of the absorbance according to eq. (9).

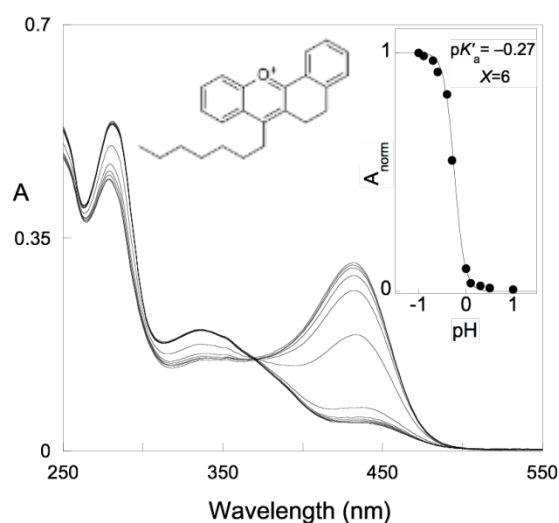


Fig. S9 – Absorption spectra of compound **5a** 2.3×10^{-5} M in the presence of 20% (w/v) Pluronic® micelles at room temperature. Fitting of the absorbance according to eq. (9).