SYNTHESIS, CHARACTERIZATION AND TESTING OF NEW D-A CYANOARENE PHOTOCATALYSTS

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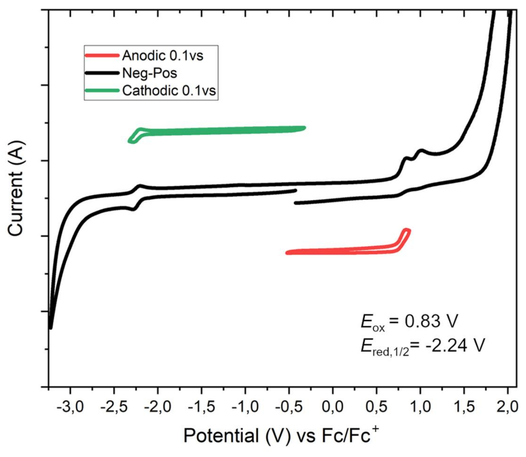
Introduction

One of the best performing donor-acceptor cyanoarene photocatalyst, commercially available **3DPA2FBN**,[1, 2] when irradiated, produces two by-products, identified by HPLC-MS analysis as deriving, respectively, from loss of one and two HF molecules.[3]

In this work, we successfully isolated the two products (**1** and **2**) as single regioisomers and assessed an optimized method to synthesize them.

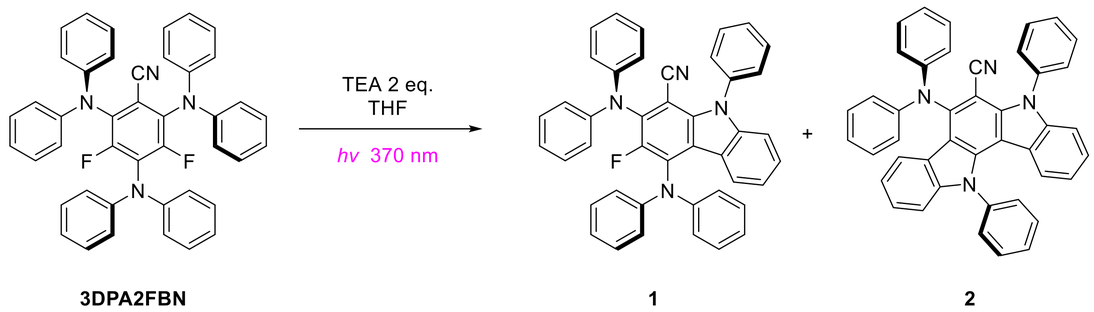
NMR and XRD studies fully elucidated the structures of these products. The photophysical properties of **1** and **2** were determined by electrochemical and spectroscopic techniques. Their catalytic activity was preliminarily assessed in suitable photocatalyzed reactivities.

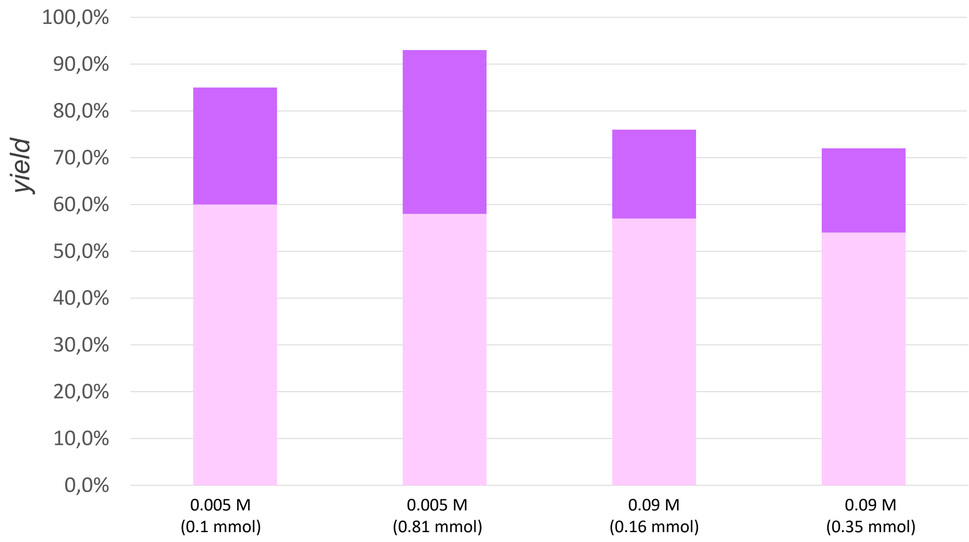
Mono-cyclized product **1**



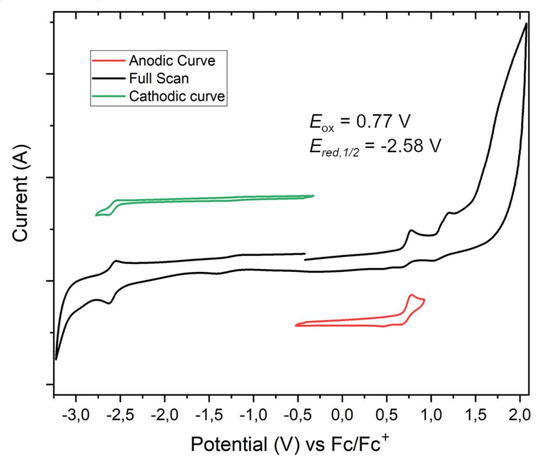
	Potential (vs SCE)
E(PC⁺/PC)	1.22 V
E((PC/PC⁻)	-1.85 V
E(PC*/PC⁻)	1.01 V
E(PC⁺/PC*)	-1.64 V

$E_{0,0}^{S1}$ = 2.86 eV



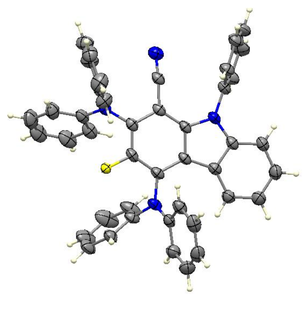


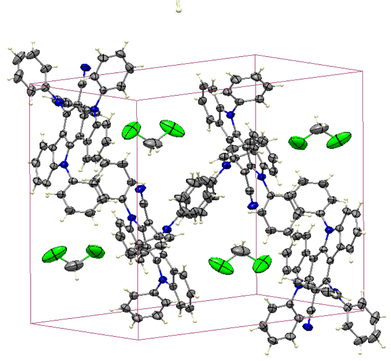
Bis-cyclized product **2**

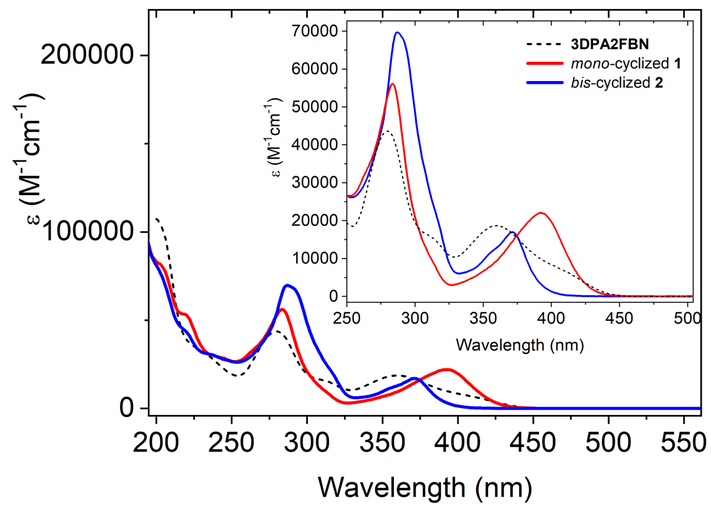


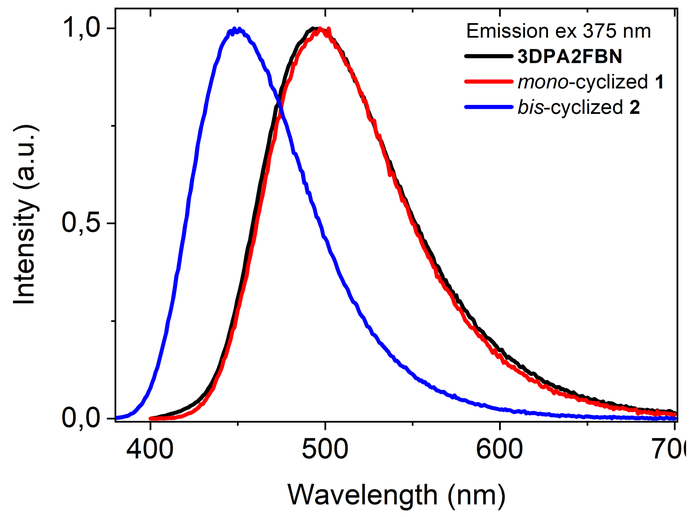
	Potential (vs SCE)
E(PC⁺/PC)	1.16 V
E((PC/PC⁻)	-2.19 V
E(PC*/PC⁻)	0.91V
E(PC⁺/PC*)	-1.94 V

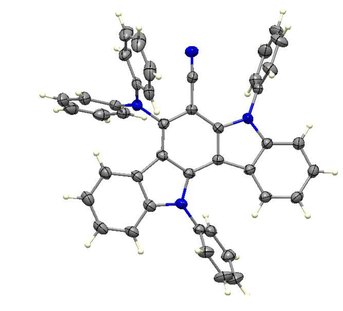
$E_{0,0}^{S1}$ = 3.10 eV

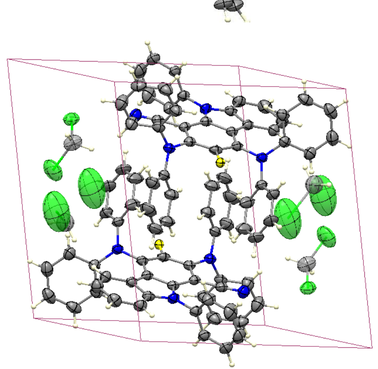


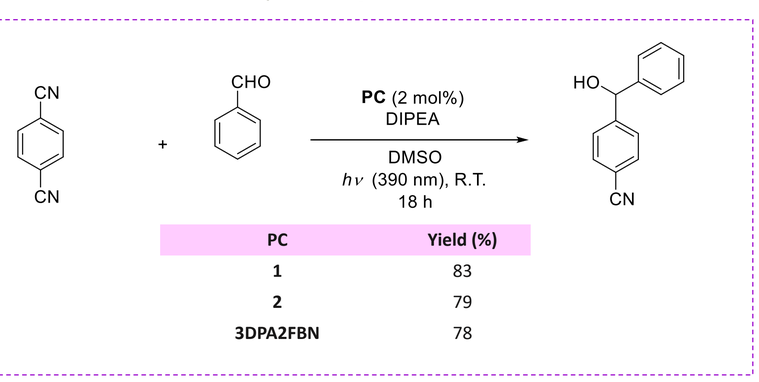




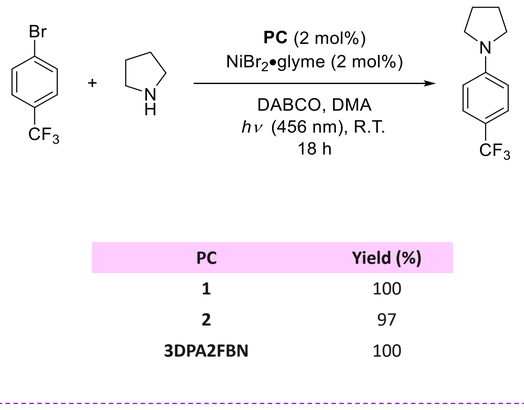




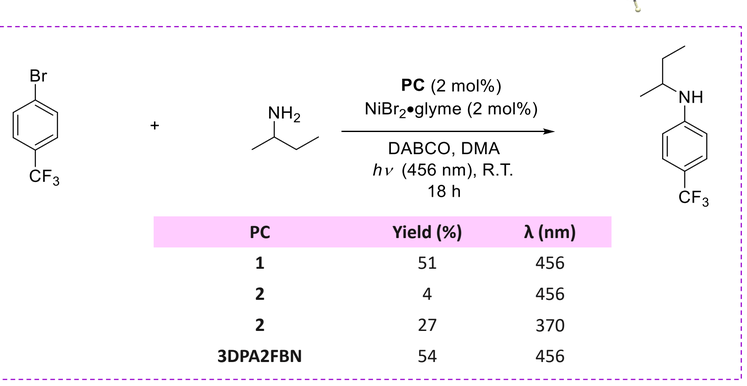




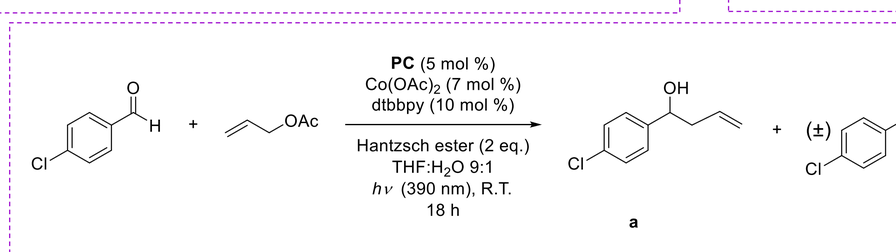
PC	Yield (%)
1	83
2	79
3DPA2FBN	78



PC	Yield (%)
1	100
2	97
3DPA2FBN	100



PC	Yield (%)	λ (nm)
1	51	456
2	4	456
2	27	370
3DPA2FBN	54	456



PC	Yield (%)	Ratio (a:b:c)
1	87	1 : 1.6 : 1.5
2	67	1.5 : 1 : 1.1
3DPA2FBN	89	1 : 1.4 : 1.6

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