

Dynamic Electrochemistry of Anthanthrone

<u>Abel Cárdenas</u>^a, Fréderic Lirette^b, José Marín-Beloqui^a, David Casanova^c, Jean-François Morin^b, Juan Casado^a

a Department of Physical Chemistry, University of Málaga, Andalucia-Tech, Campus de Teatinos s/n, 29071 Málaga, Spain

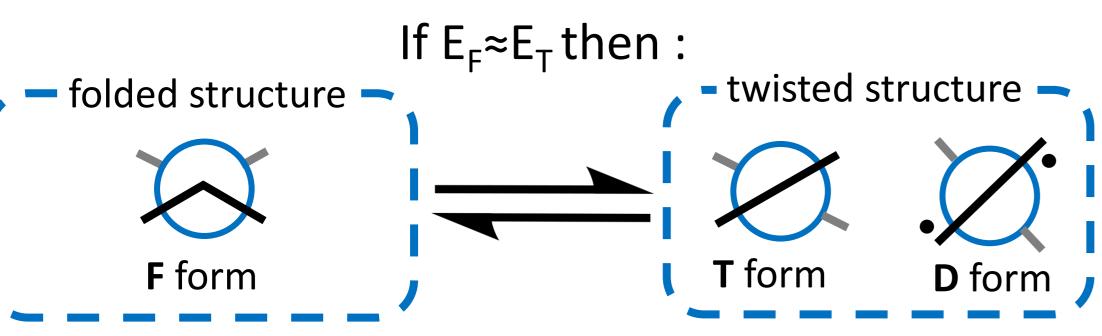
- b Département de Chimie, Université Laval, 1045 Ave de la Médecine, Québec, Canada G1V 0A6
- c IKERBASQUE Basque Foundation for Science (DC) & Donostia International Physics Center, Paseo Manuel de Lardizabal, 4, 20018 Donostia-San Sebastián, Euskadi, Spain

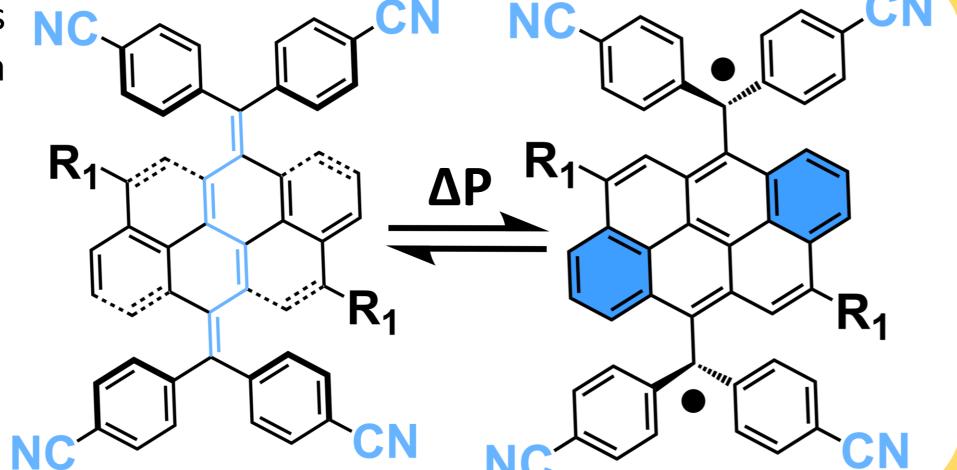
abel@uma.es



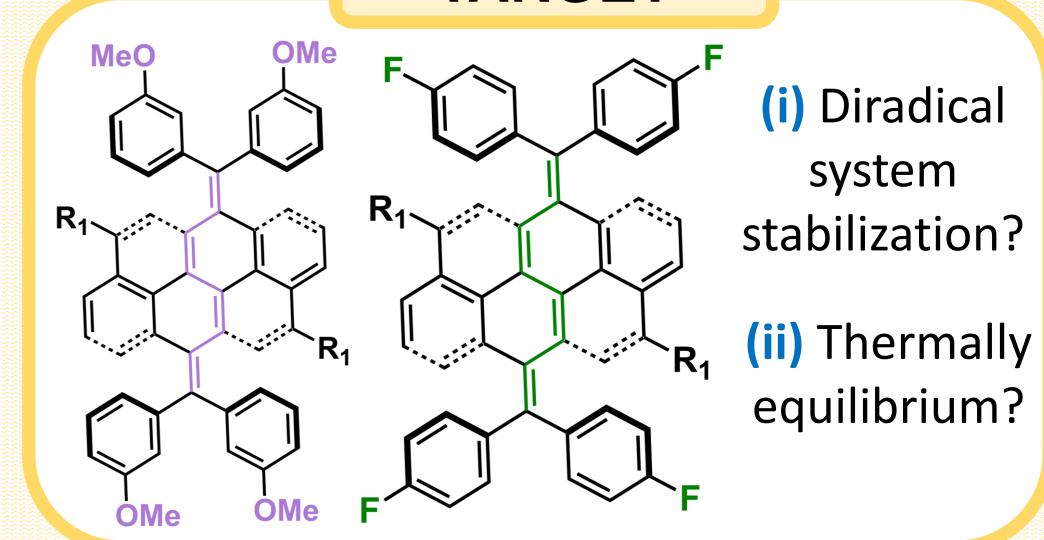
INTRODUCTION

Overcrowded ethylenes (OCEs), in which the C=C double bond is NC surrounded by bulky substituents. OCEs are forced to adopt a folded (**F**), Twisted close shell (**T**) or Twisted dirradical (**D**) form.





TARGET



ELECTRONIC STRUCTURE CHARACTERIZATION

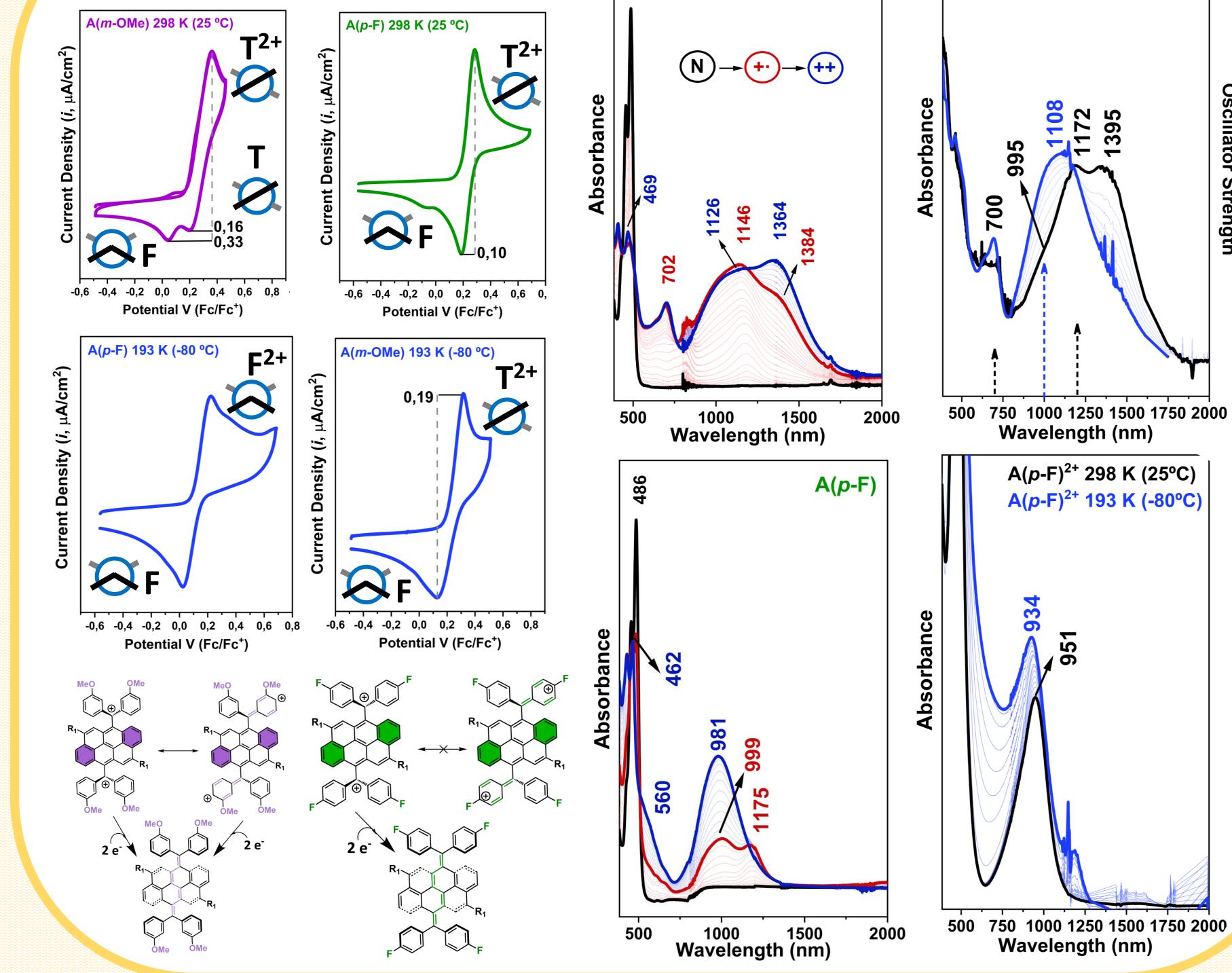
NEUTRAL SPECIES A(meta-OMe) cillator rel (Kcal/mol) TOS SOS 500 **SOS** 2,5 Wavelength (nm) **Emision Room** HOMO HOMO **Emision Low T Emision Low** 1 -1,0 **Excitation** -1,5 **F** form **D** form **F** form **D** form Wavelength (nm)

A(m-OMe)²⁺ 298 K (25°C)

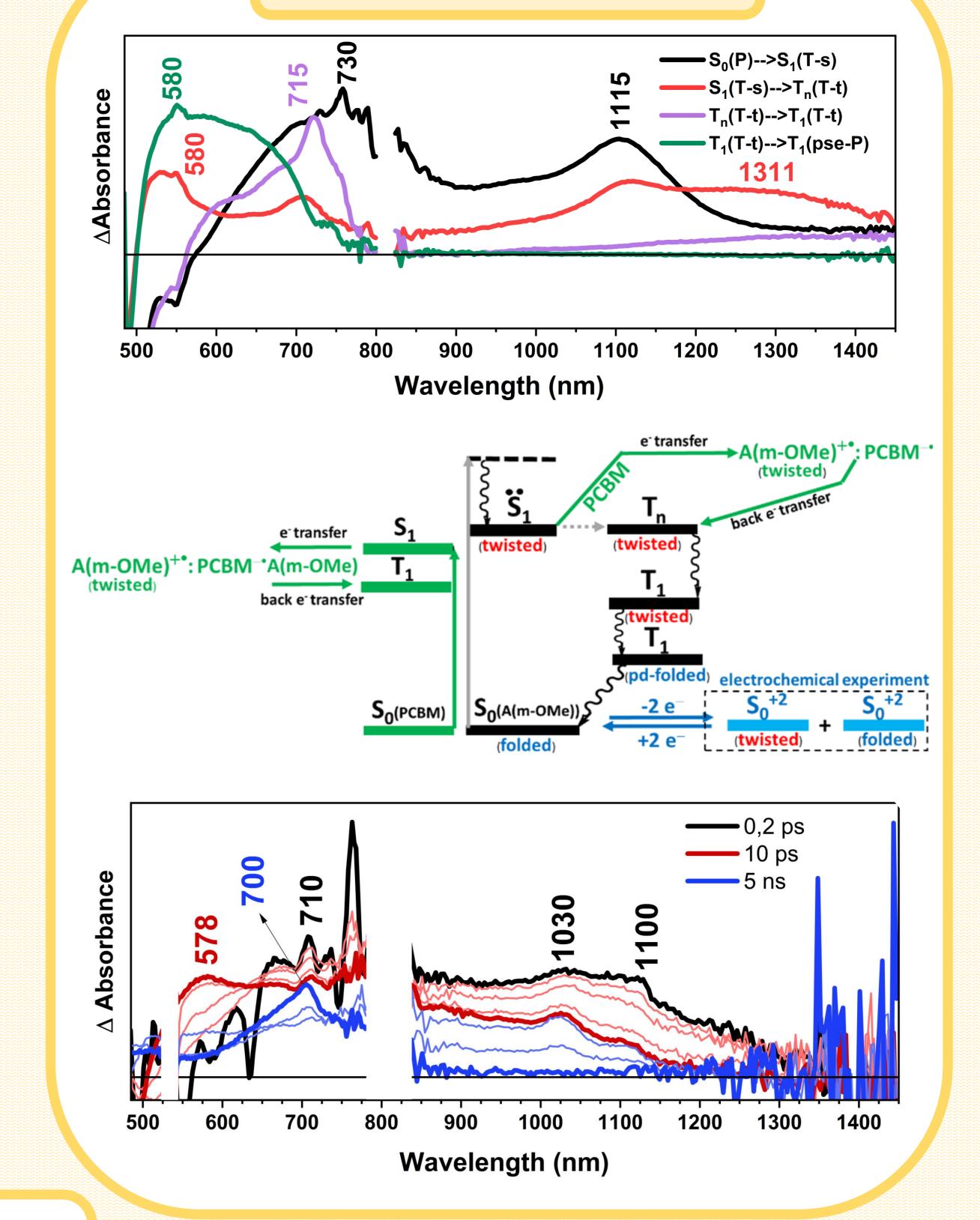
 $A(m-OMe)^{2+}$ 193 K (-80°C)

A(m-OMe)

CHARGED SPECIES



TRANSIENT SPECIES



CONCLUSIONS

(i) In the neutral state, there is not a diradical system stabilization but, the nearness between twisted dirradical triplet state and ground state allow the formation of an open shell system.

(ii) There is a dynamic redox in A(*meta-OMe*), promoted by thermal equilibrium at room temperature between both conformations.