

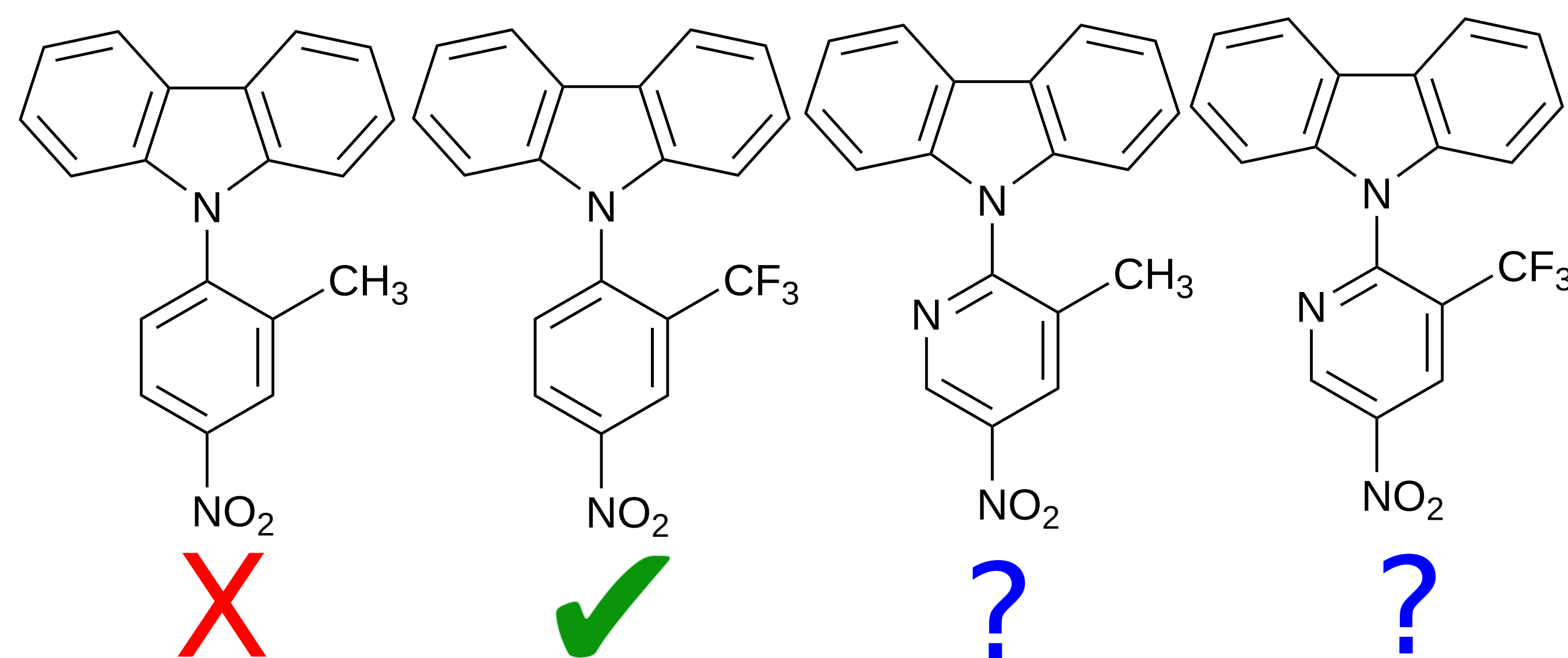
# Exploring the excited state character of nitroarylcarbazole derivatives using wavefunction analysis

P. Kimber<sup>1</sup>, I. A. Wright<sup>1</sup>, F. Plasser<sup>1</sup><sup>1</sup>Department of Chemistry, Loughborough University, UK

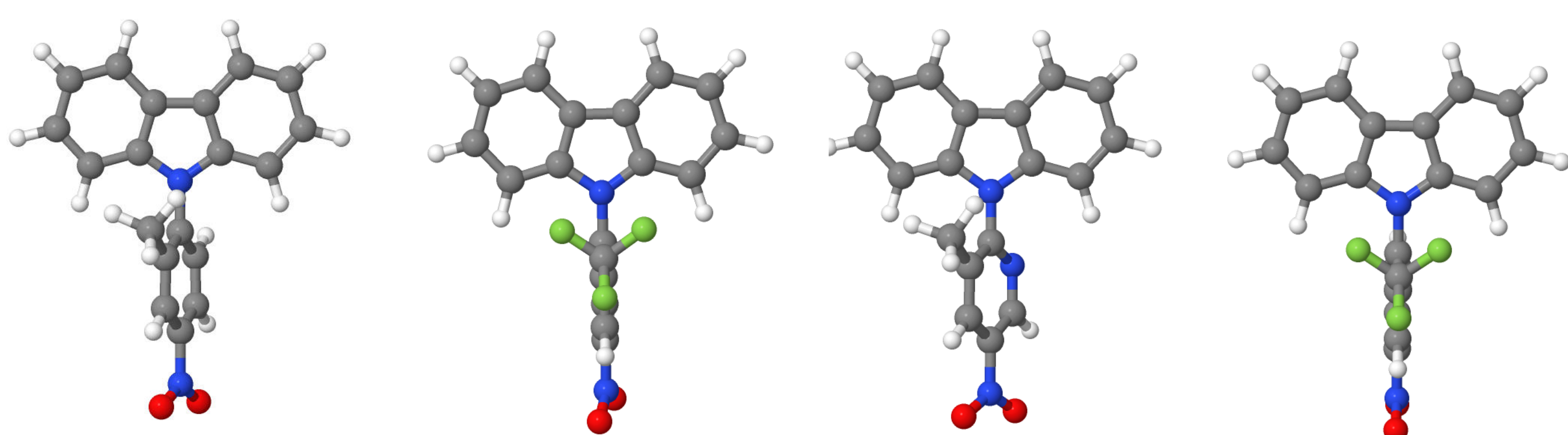
## Introduction

- Nitroarylcarbazoles can display aggregation induced emission behaviour<sup>1</sup>
- Can we understand this behaviour in terms of the electronic transitions which occur on excitation?

## Solid state emissive?



## 1. Ground state optimised structures

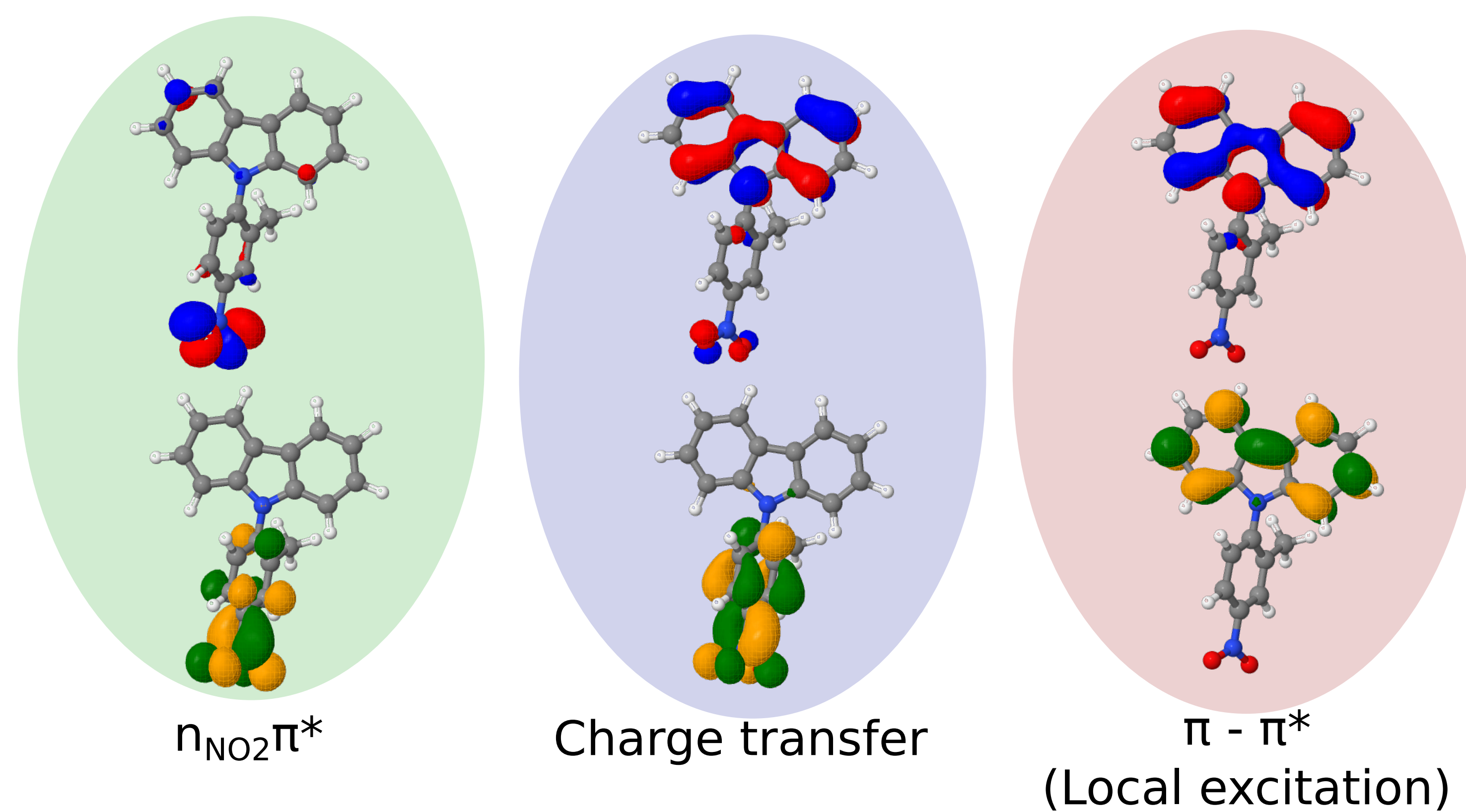


Methyl containing aryl groups → twisted

Trifluoro containing aryl groups → orthogonal

Calculate vertical excitations and use fragment decomposition to analyse the excited states

## 2. Excited state characterisation



## 4. PhCF<sub>3</sub> - a closer look

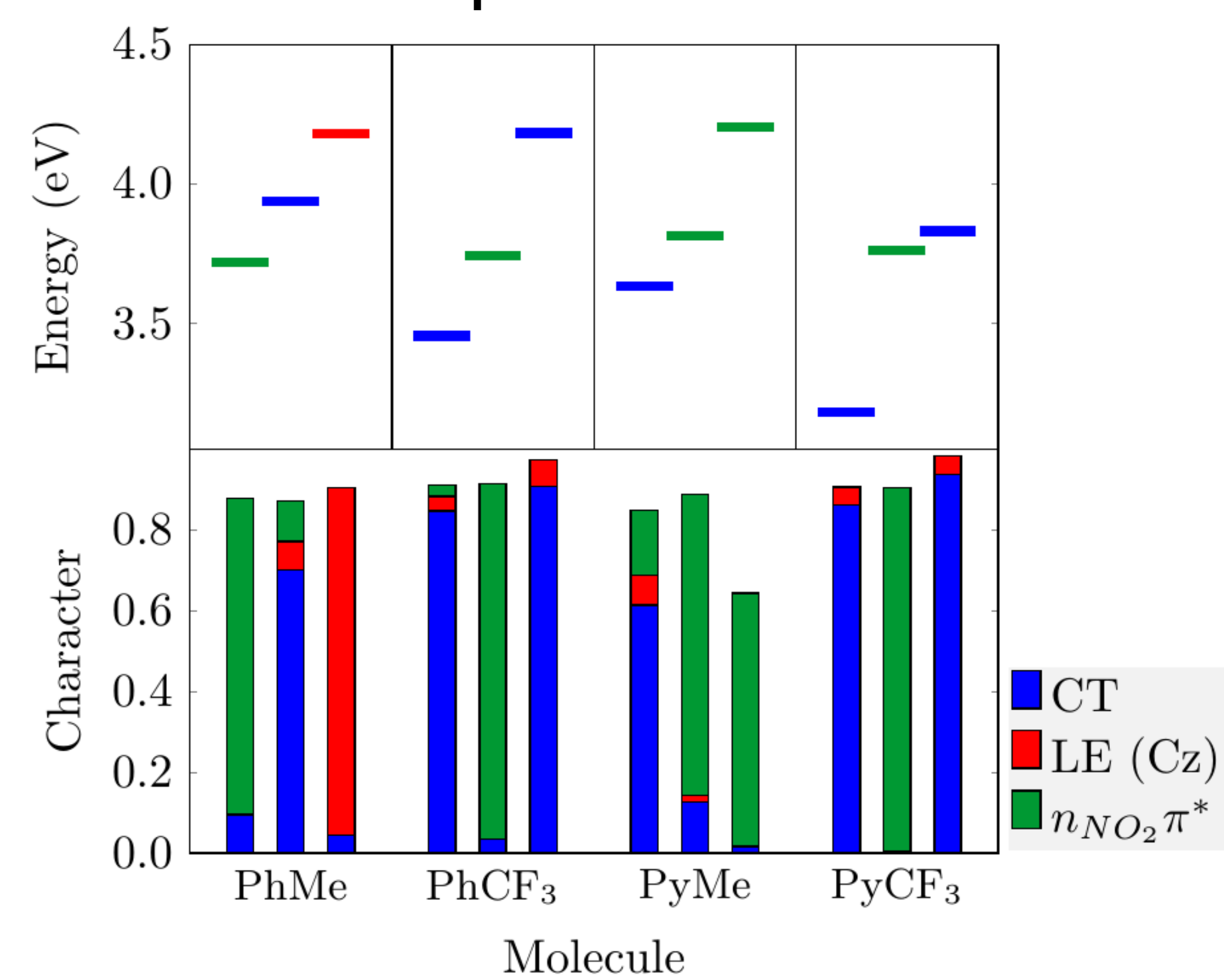
State	$\Delta E$ (eV)	f	CT	Character
$S_1$	3.455	0.000	0.887	CT
$S_2$	3.744	0.000	0.045	$n_{NO_2}\pi^*$
$S_3$	4.183	0.000	0.932	CT

Zero oscillator strength but solid state emissive - how?

Rotation from the orthogonal conformation to a planar one.



## 3. Bar representation



## 5. Conclusions

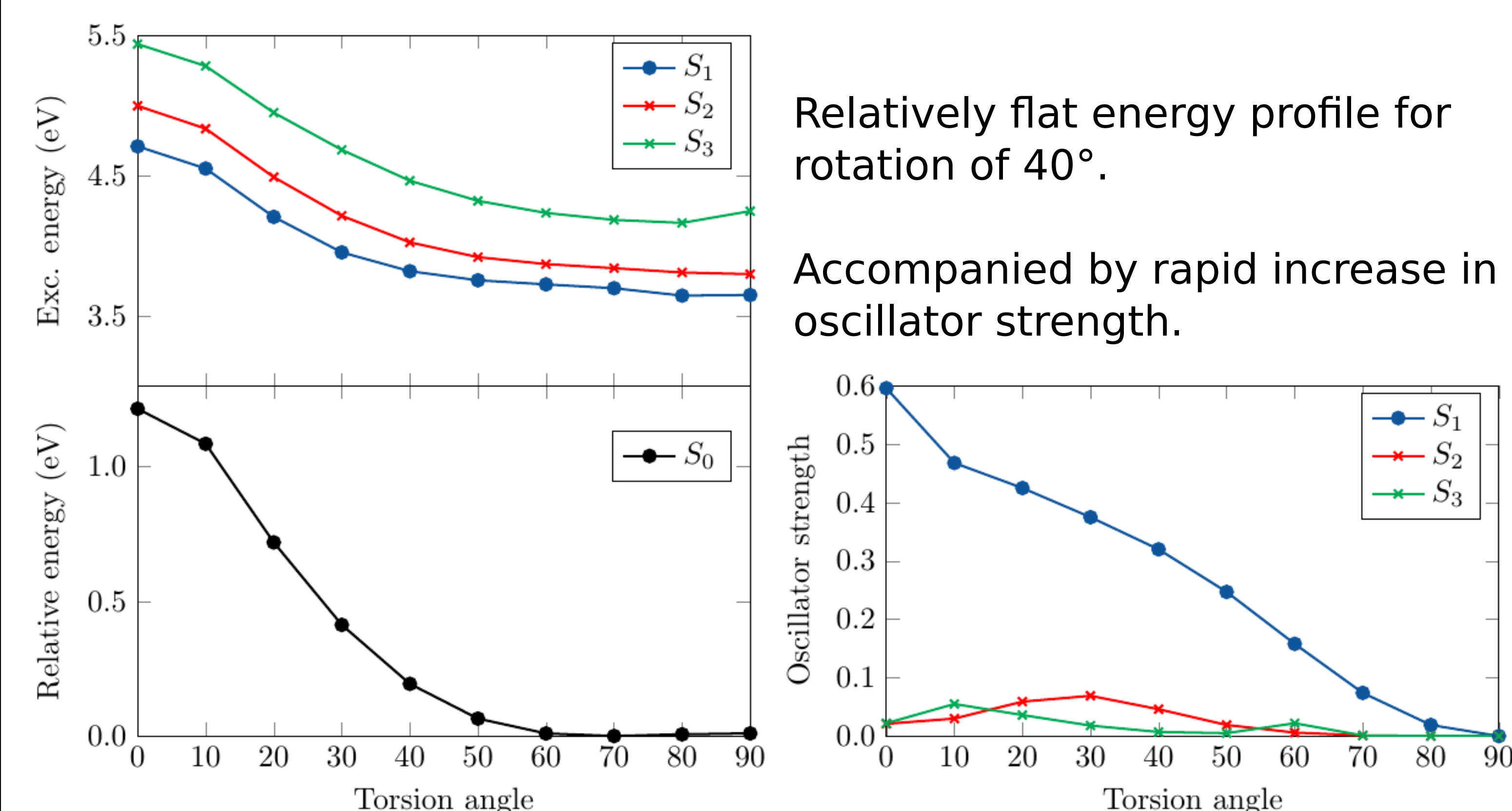
We propose that provided:

- The barrier to reach a conformation with appreciable oscillator strength is small
- The first excited state is a charge transfer state

The molecule will be solid state emissive.

## Computational details

Turbomole 7.4 using MP2/def2-SV(P) for geometry optimisations and ADC(2)/def2-SV(P) for vertical excitations.

TheoDORE 2.0.2 for wavefunction analysis and decomposition of excited states.<sup>2</sup>

Relatively flat energy profile for rotation of 40°.

Accompanied by rapid increase in oscillator strength.

## REFERENCES

- Mater. Chem. Front., 2017,1, 1125-1129. DOI: 10.1039/C6QM00343E
- F. Plasser, TheoDORE: a package for theoretical density, orbital relaxation and exciton analysis; available from <http://theodore-qc.sourceforge.net/>

## ACKNOWLEDGEMENTS

I would like to thank Dr Felix Plasser for his ongoing support with this work. Additional thanks to Dr Iain Wright for helpful discussions at the beginning of this project.



## CONTACT INFORMATION

Department of Chemistry  
Loughborough University  
Leicestershire LE11 3TU UK  
E: P.Kimber@lboro.ac.uk  
W: fplasser.sci-public.lboro.ac.uk