Solavation effect observed on a molecule deposited on an argon cluster

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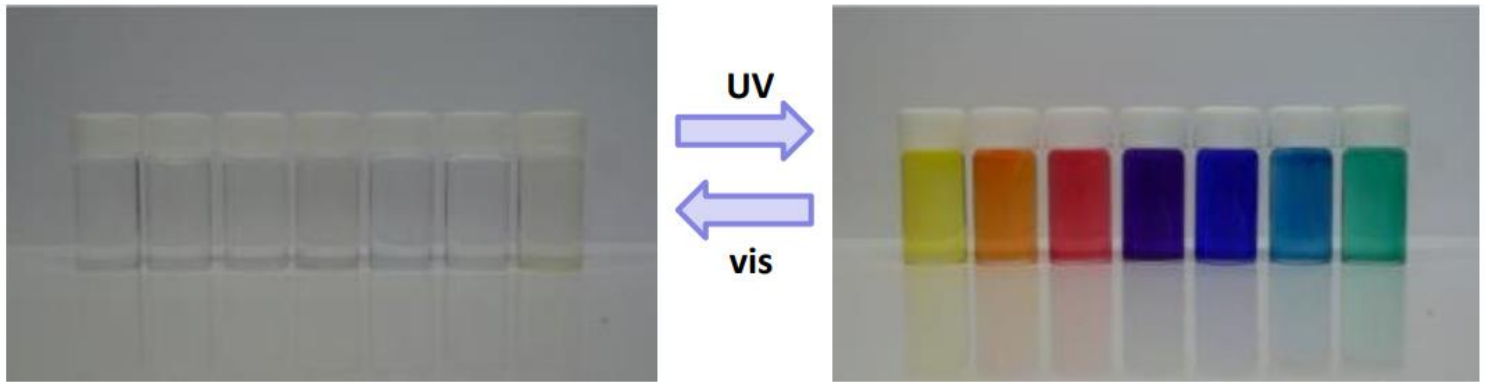
Université Paris-Saclay
ISMO - Institut des Sciences Moléculaires d'Orsay
LIDYL - Laboratoire Interactions, Dynamiques et Lasers

ICPA-12, September 29th 2022

Photochromism



Kobatake, S., & Irie, M. (2004). Single-crystalline photochromism of diarylethenes. *Bulletin of the Chemical Society of Japan*, *77*(2), 195-210.

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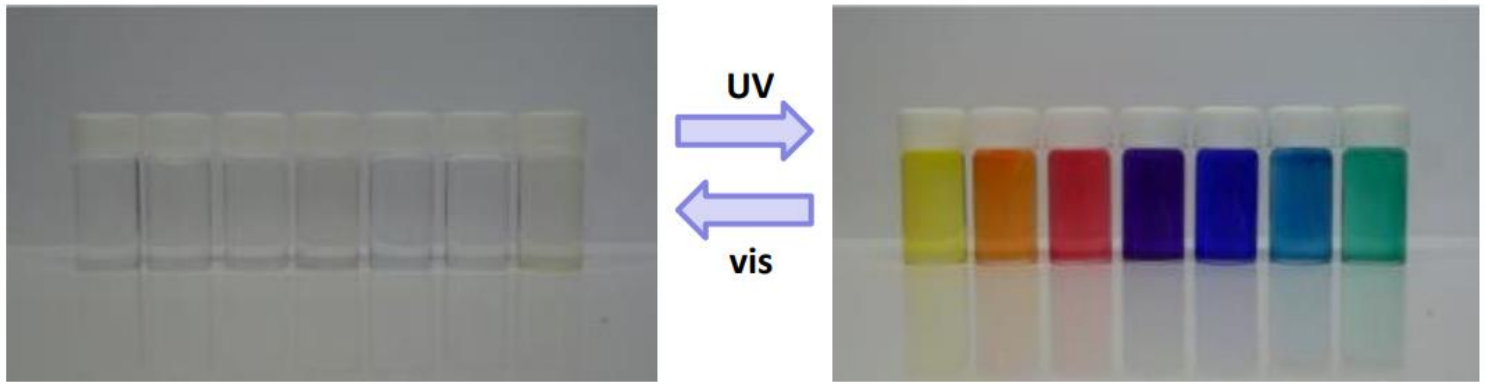
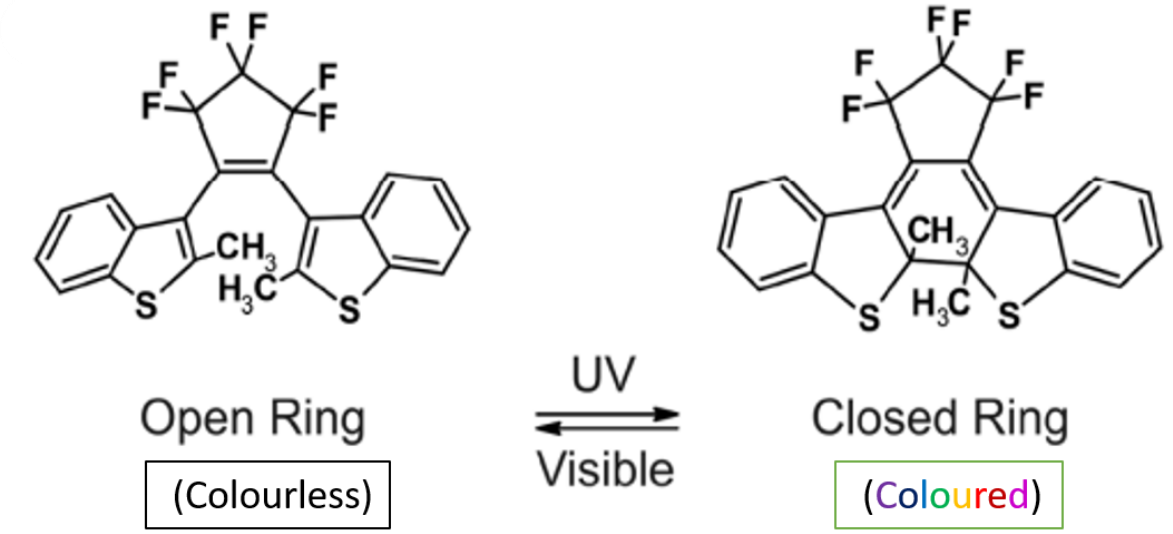


Class of dithienylethene molecule



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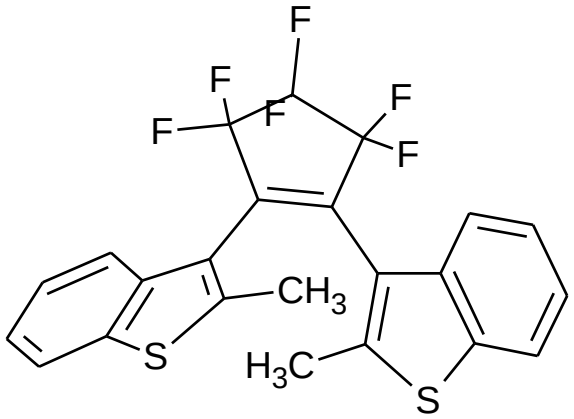
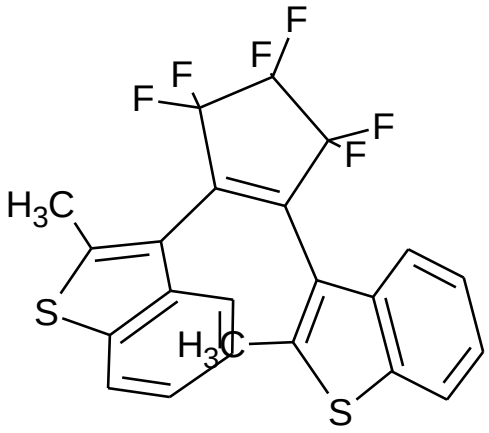
Dithienylethene molecule : open ring isomer

Anti-Parallel

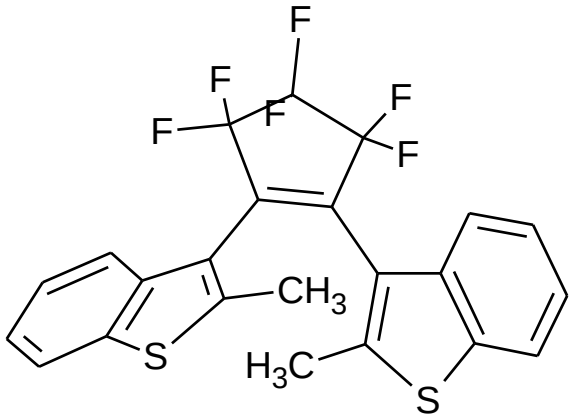


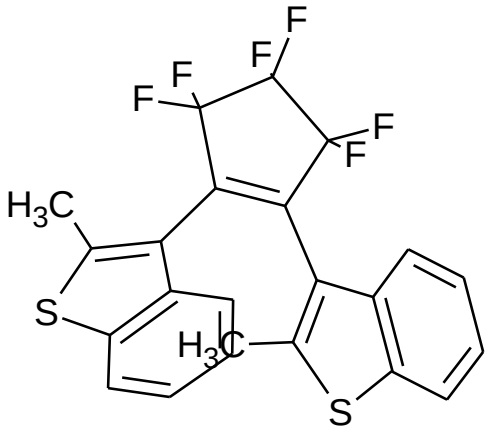


Parallel

Dithienylethene molecule : open ring isomer

Anti-Parallel





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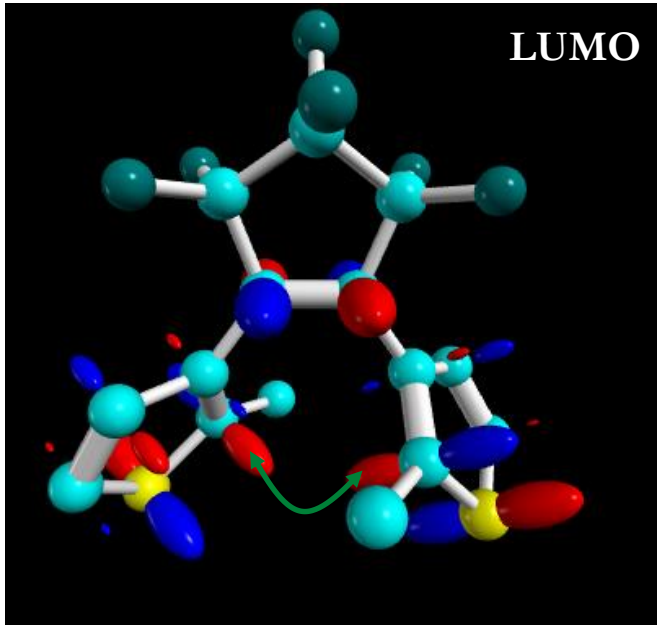
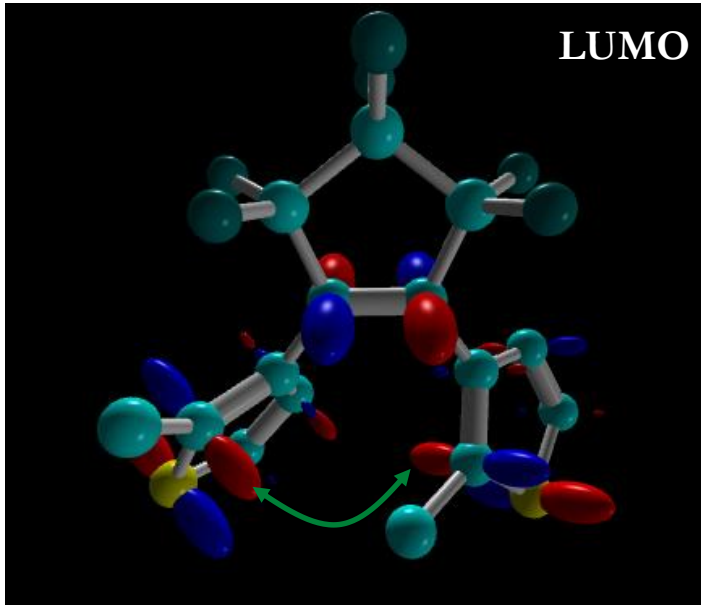
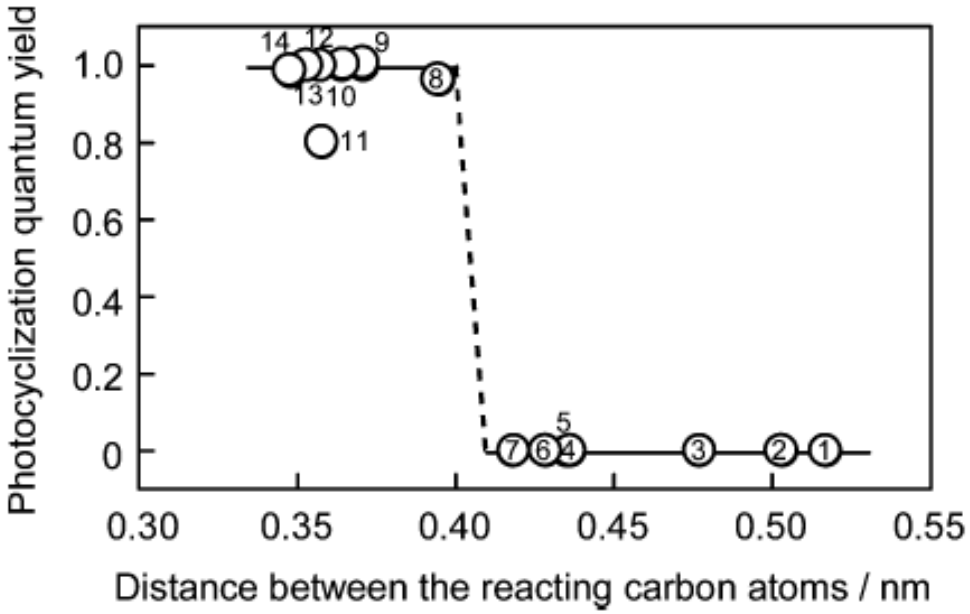




Two compounds



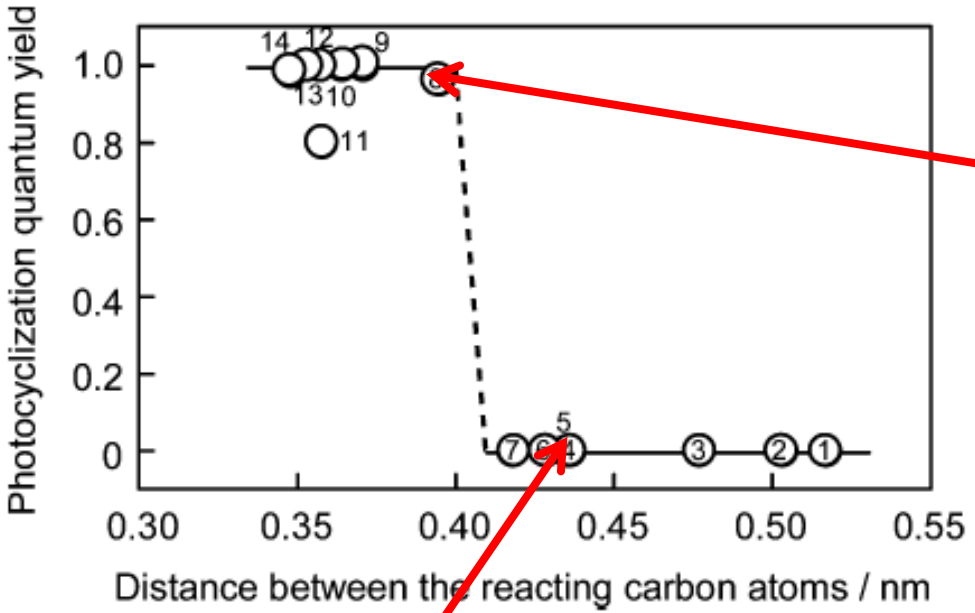
Crystal : only anti-parallel

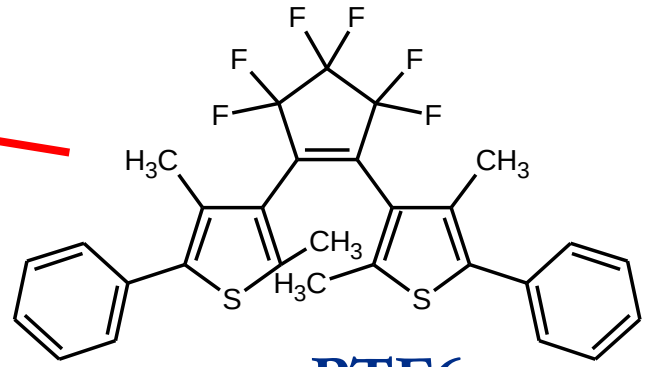
Single-crystalline photochromism of diarylethenes: reactivity–structure relationship†

Seiya Kobatake,[a] Kingo Uchida,[b] Eriko Tsuchida[b] and Masahiro Irie*[a]

Chemical Communications 23, 2804 (2002).

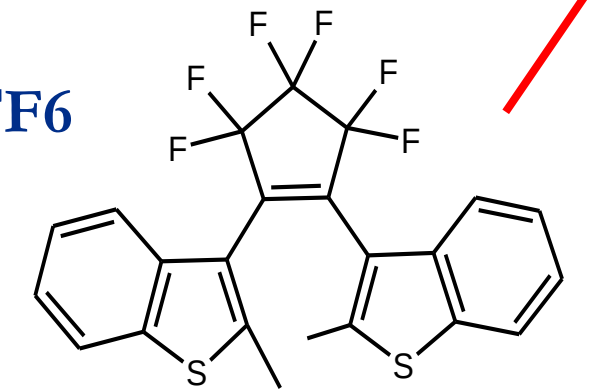
Two compounds





PTF6

BTF6



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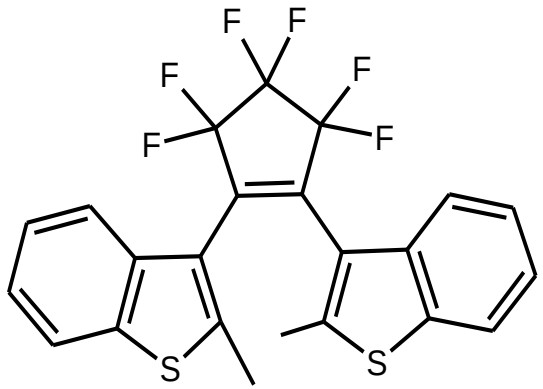
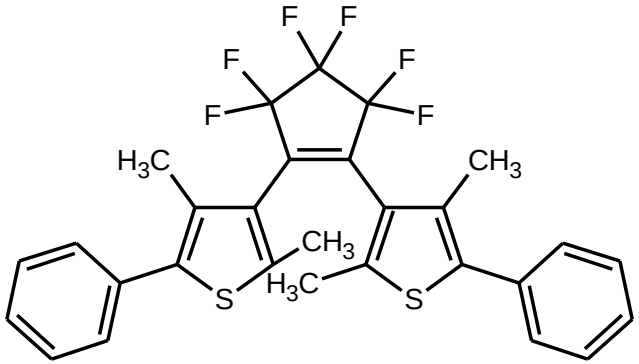


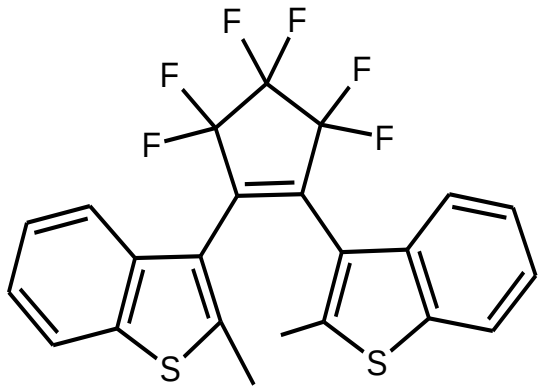
PTF6



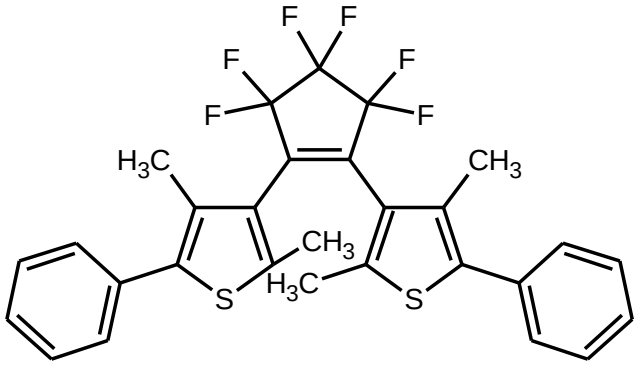
Kobatake, S.; Irie, M. *Bull. Chem. Soc. Jpn. 2004, 77, 195.*
Uchida, K.; Tsuchida, E.; Aoi, Y.; Nakamura, S.; Irie, M. Chemistry Letters 1999, 28, 63.
Irie, M.; Lifka, T.; Kobatake, S.; Kato, N. J. Am. Chem. Soc 2000, 122, 4871.
Kobatake, S.; Uchida, K.; Tsuchida, E.; Irie, M. Chemical Communications 2002, 2804.

Two compounds

BTF6



PTF6



	BTF6	PTF6
$\Phi(O \rightarrow C)$ In Crystal	0	0.96 (286 nm)
AP : P in hexane RT	65 : 35	50 : 50
$\Phi(O \rightarrow C)$ In hexane	0.35 (313 nm)	0.46 (313 nm)
$\Phi(C \rightarrow O)$ In hexane	0.35 (517 nm)	0.015 (618 nm)

Kobatake, S.; Irie, M. *Bull. Chem. Soc. Jpn. 2004, 77, 195.*
Uchida, K.; Tsuchida, E.; Aoi, Y.; Nakamura, S.; Irie, M. Chemistry Letters 1999, 28, 63.
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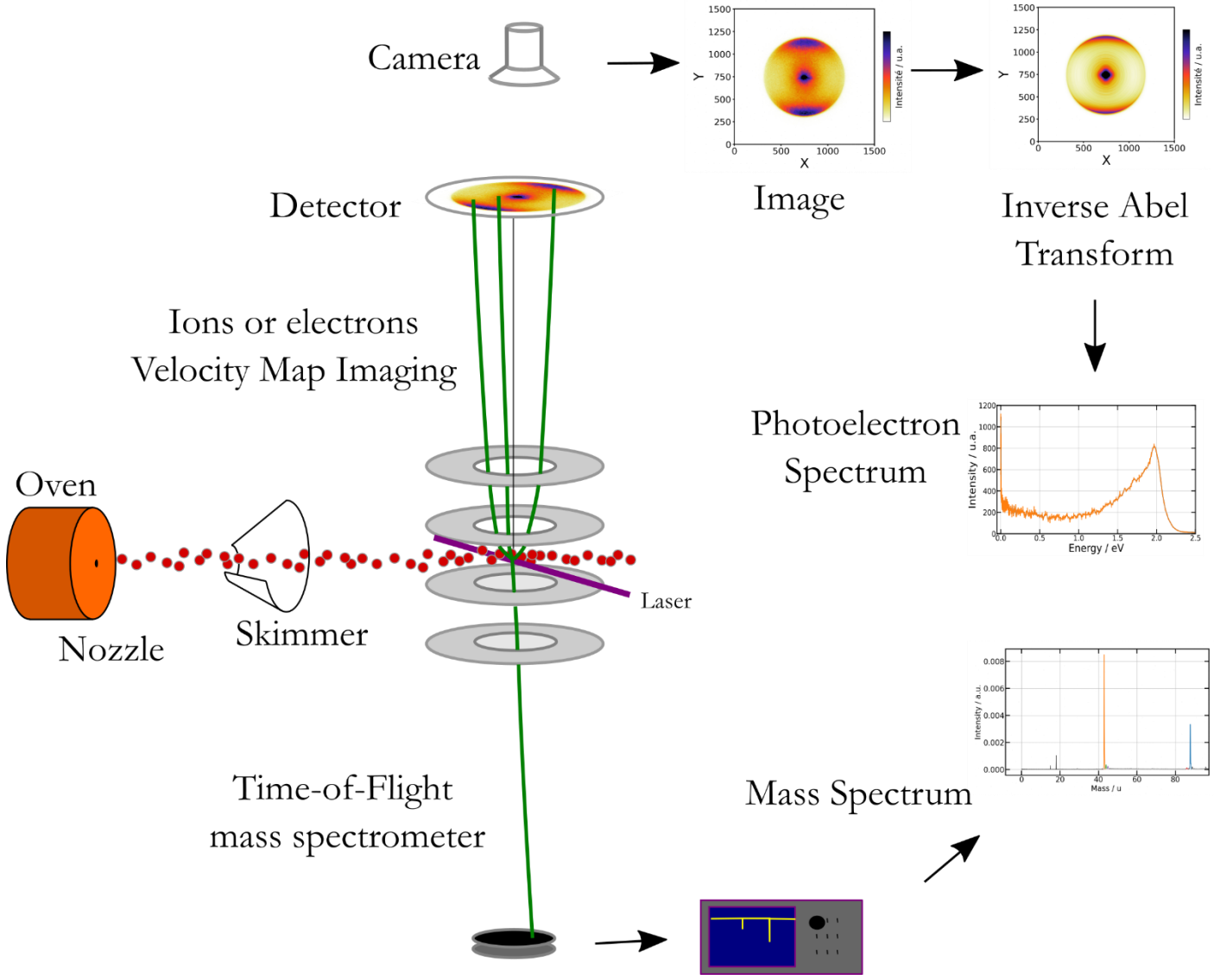
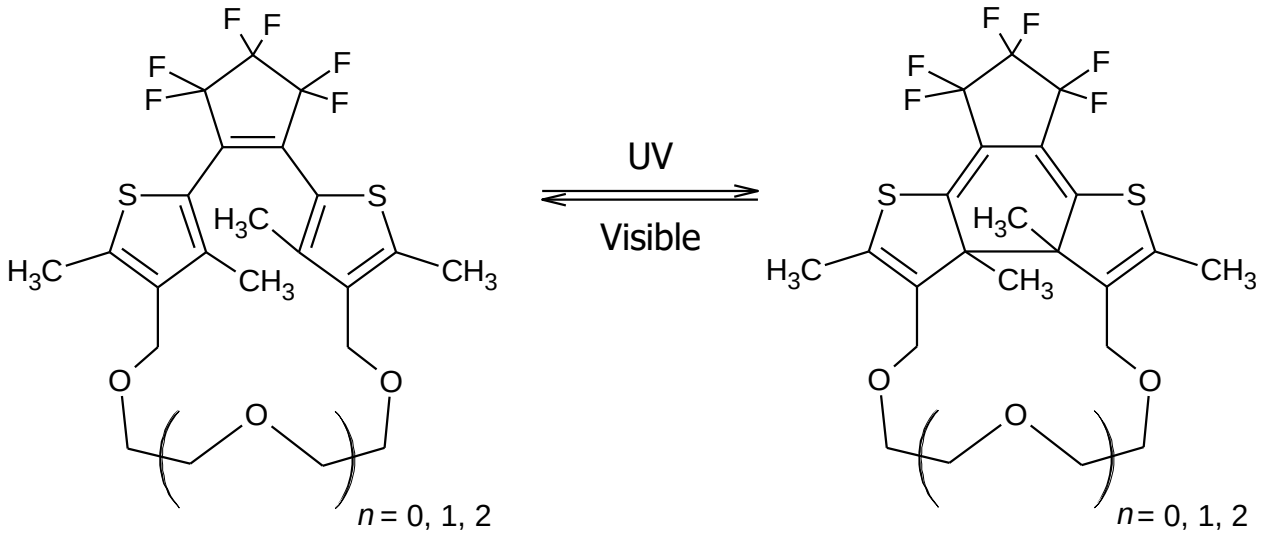
Experimental Setup



SLIC fs 20 Hz laser facility
800 nm, 2 mJ, 60 fs
266 nm, 200 µJ, 100 fs

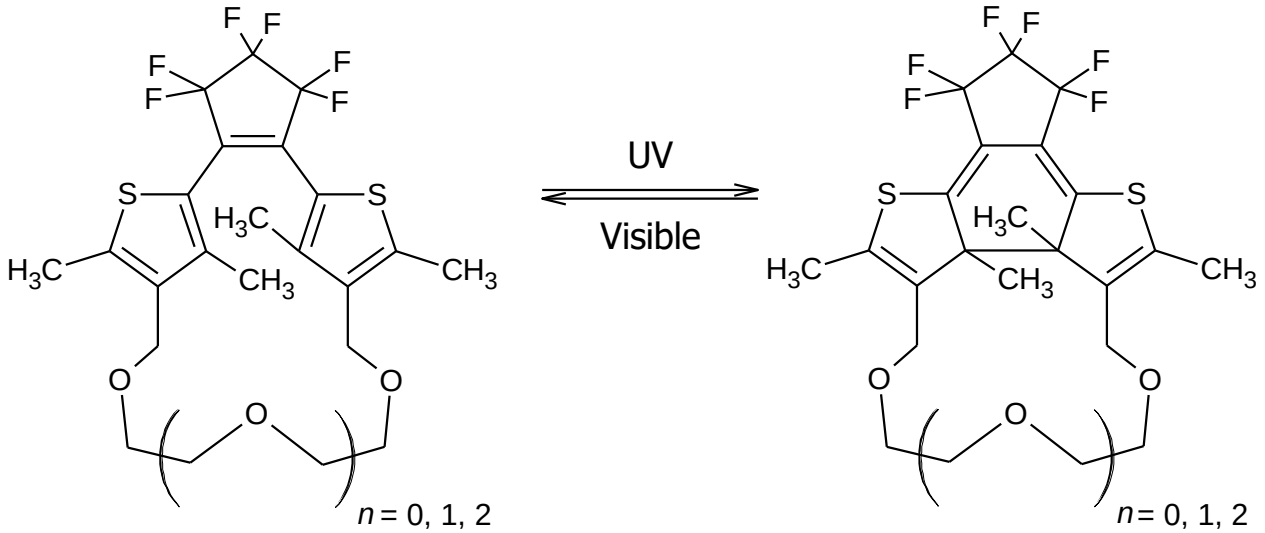
ISMO fs 3 kHz laser
800nm, 3.5 mJ, 35 fs
TOPAS, 240 -800 nm, 20 µJ, 70 fs

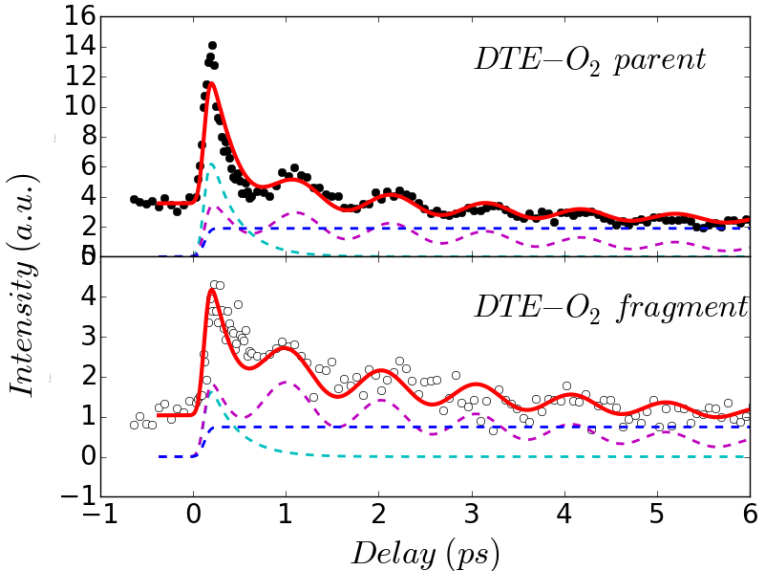
Former studies



Lietard, A.; Piani, G.; Poisson, L.; Soep, B.; Mestdagh, J. M.; Aloise, S.; Perrier, A.; Jacquemin, D.; Takeshita, M. *Phys. Chem. Chem. Phys. 2014, 16, 22262.*

Former studies





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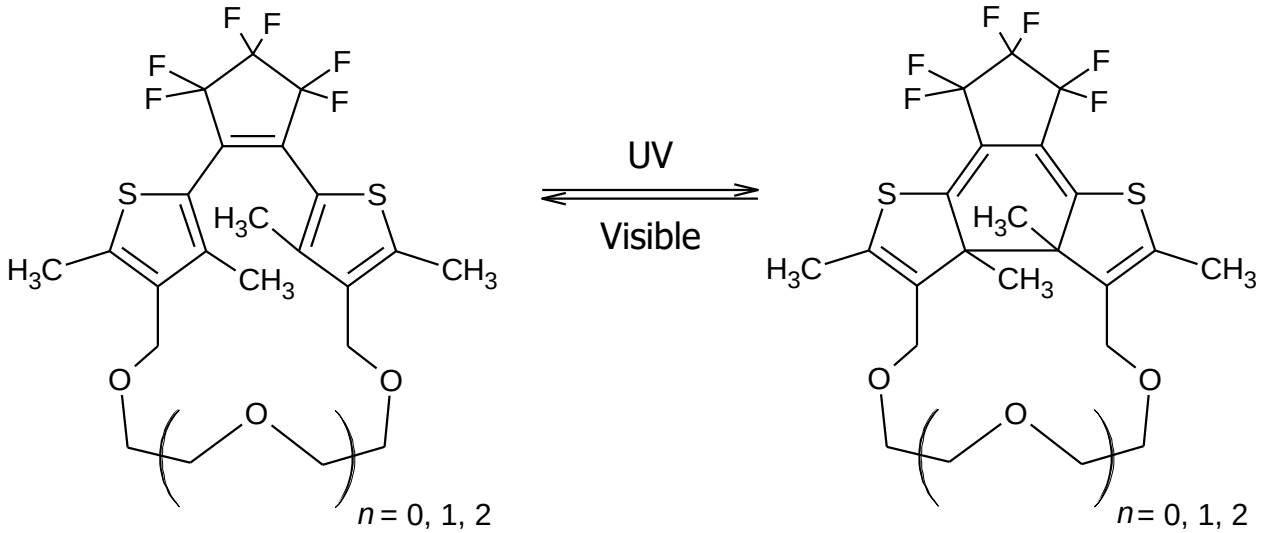

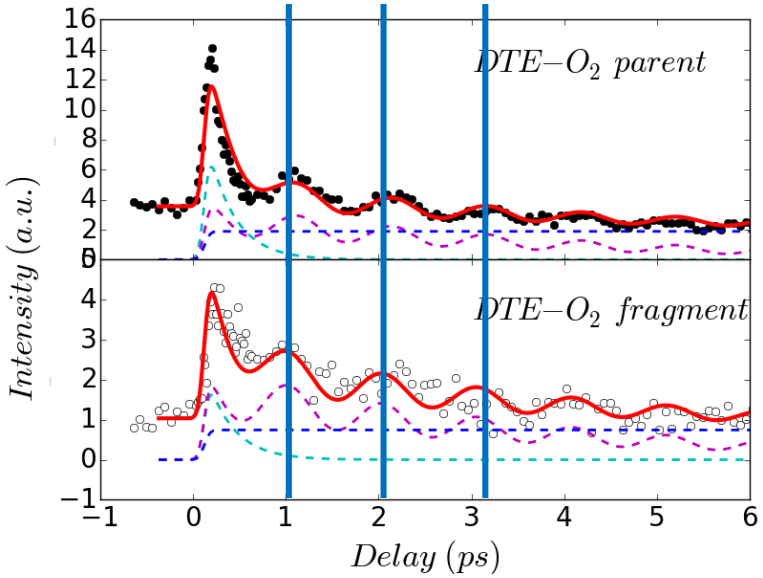

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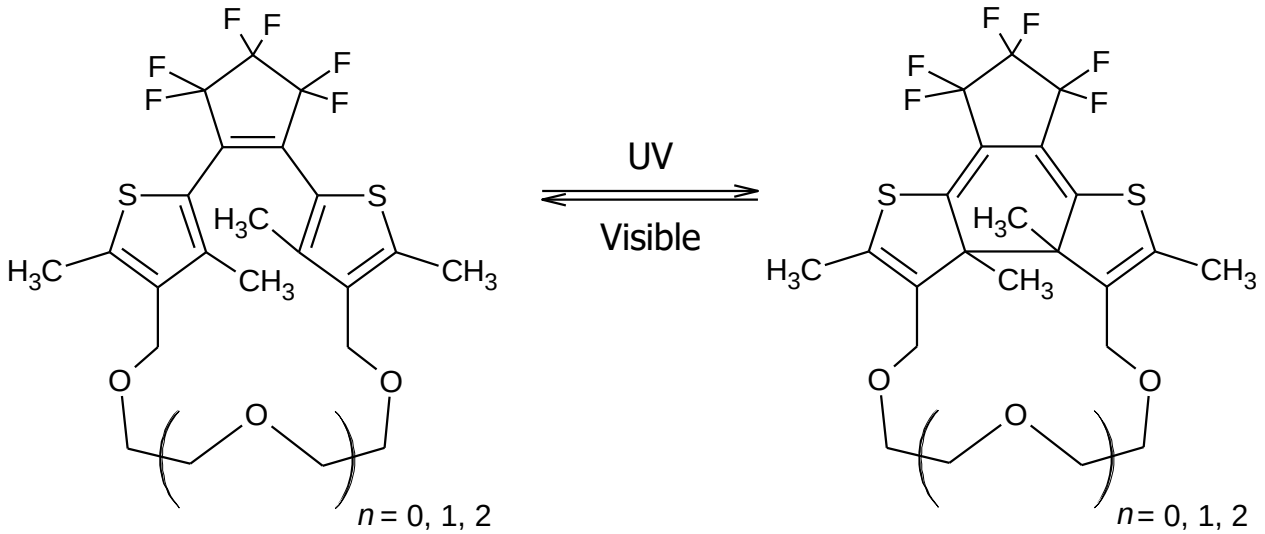

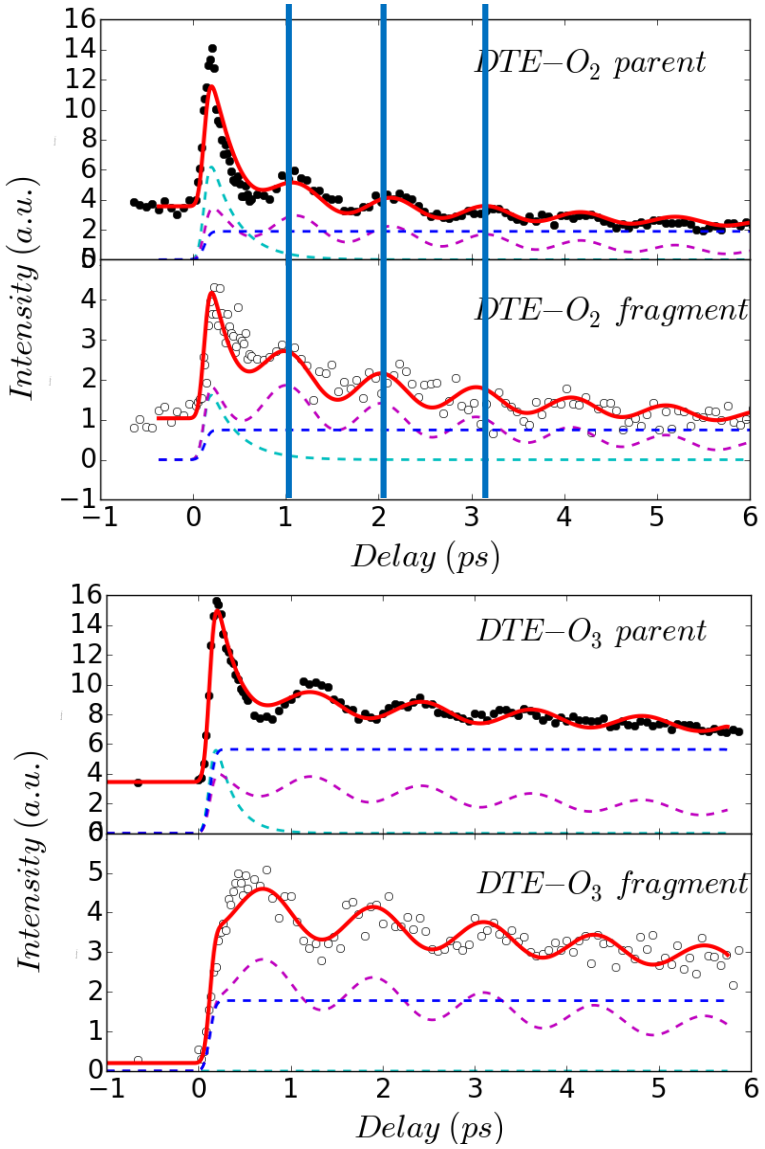

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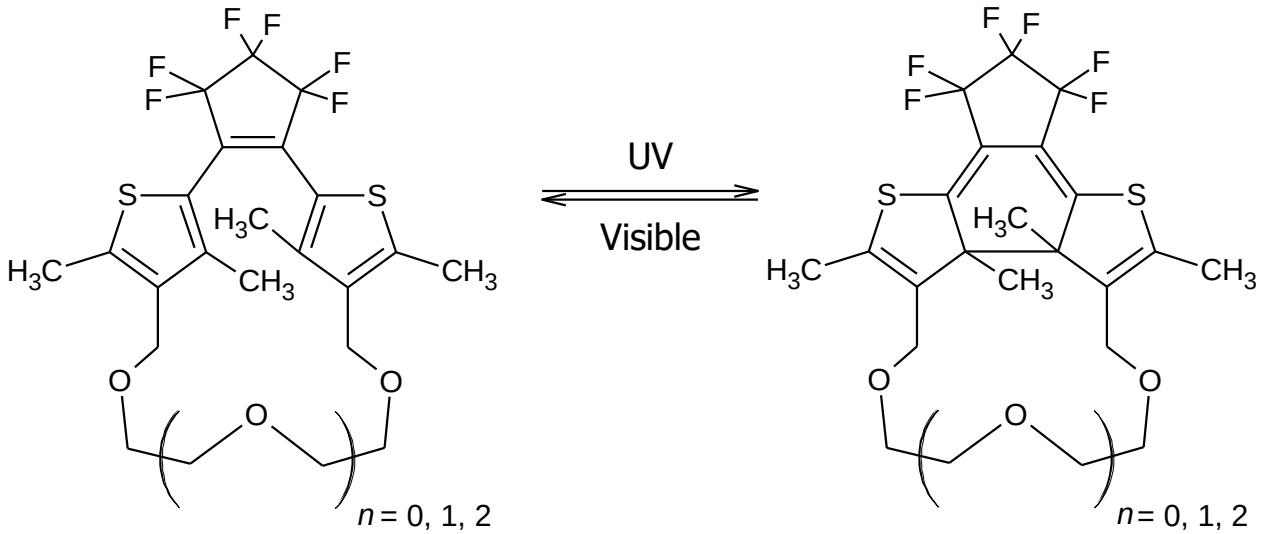

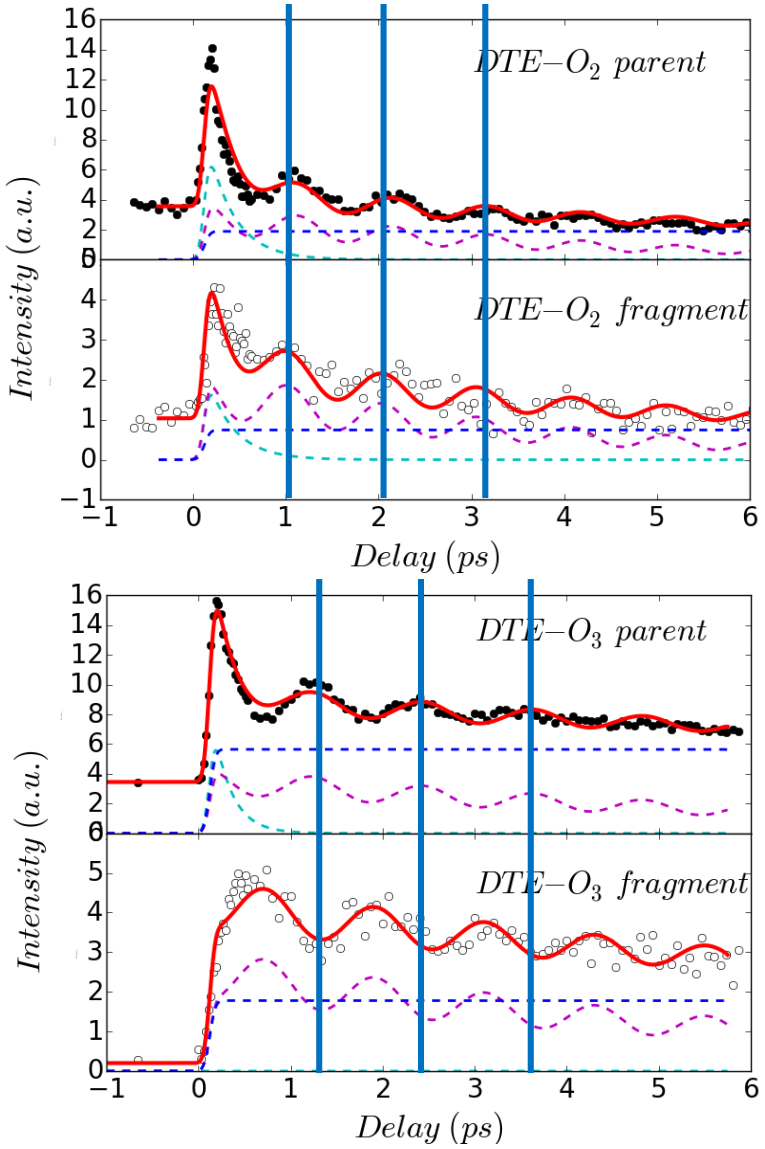

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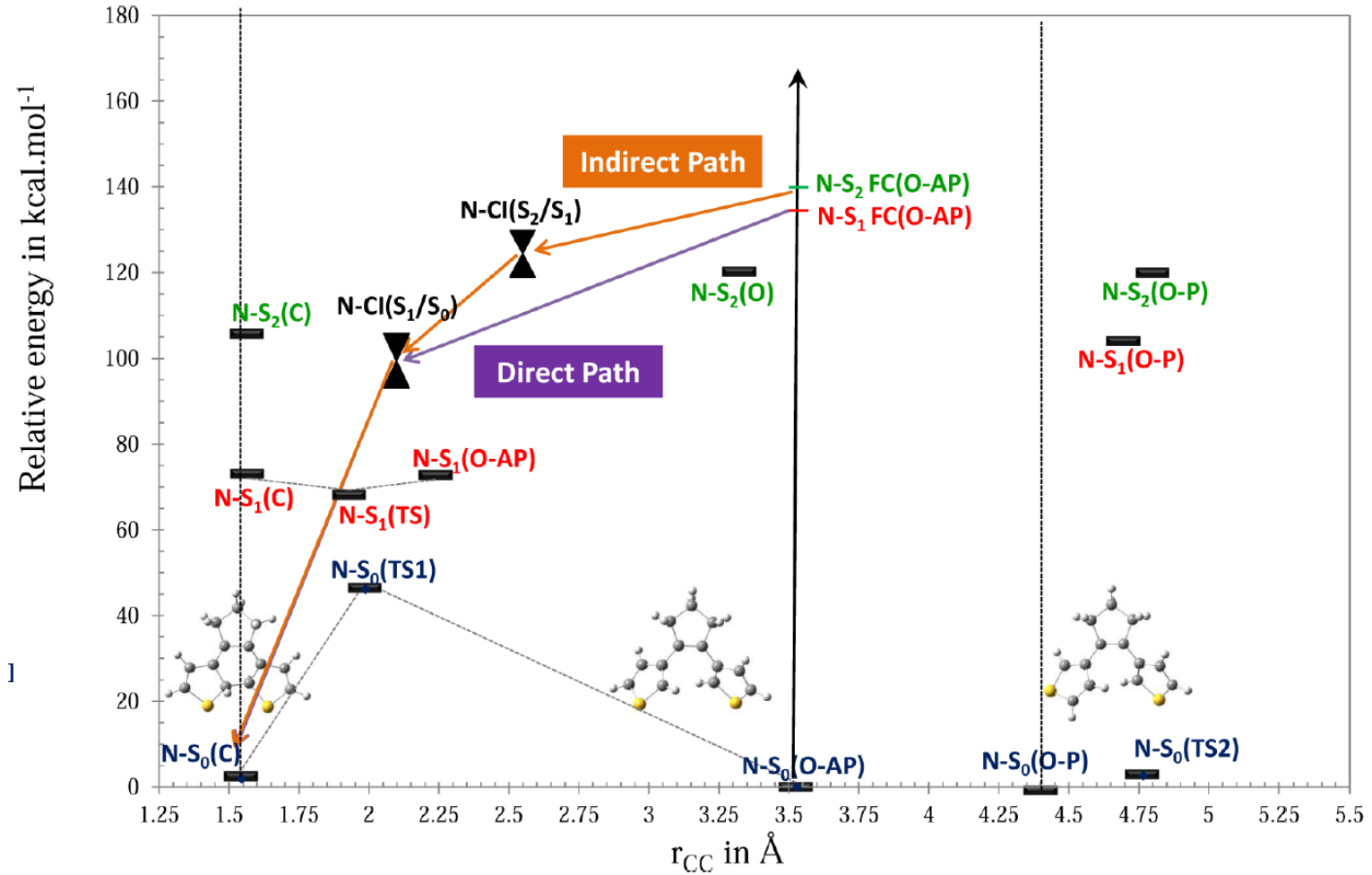
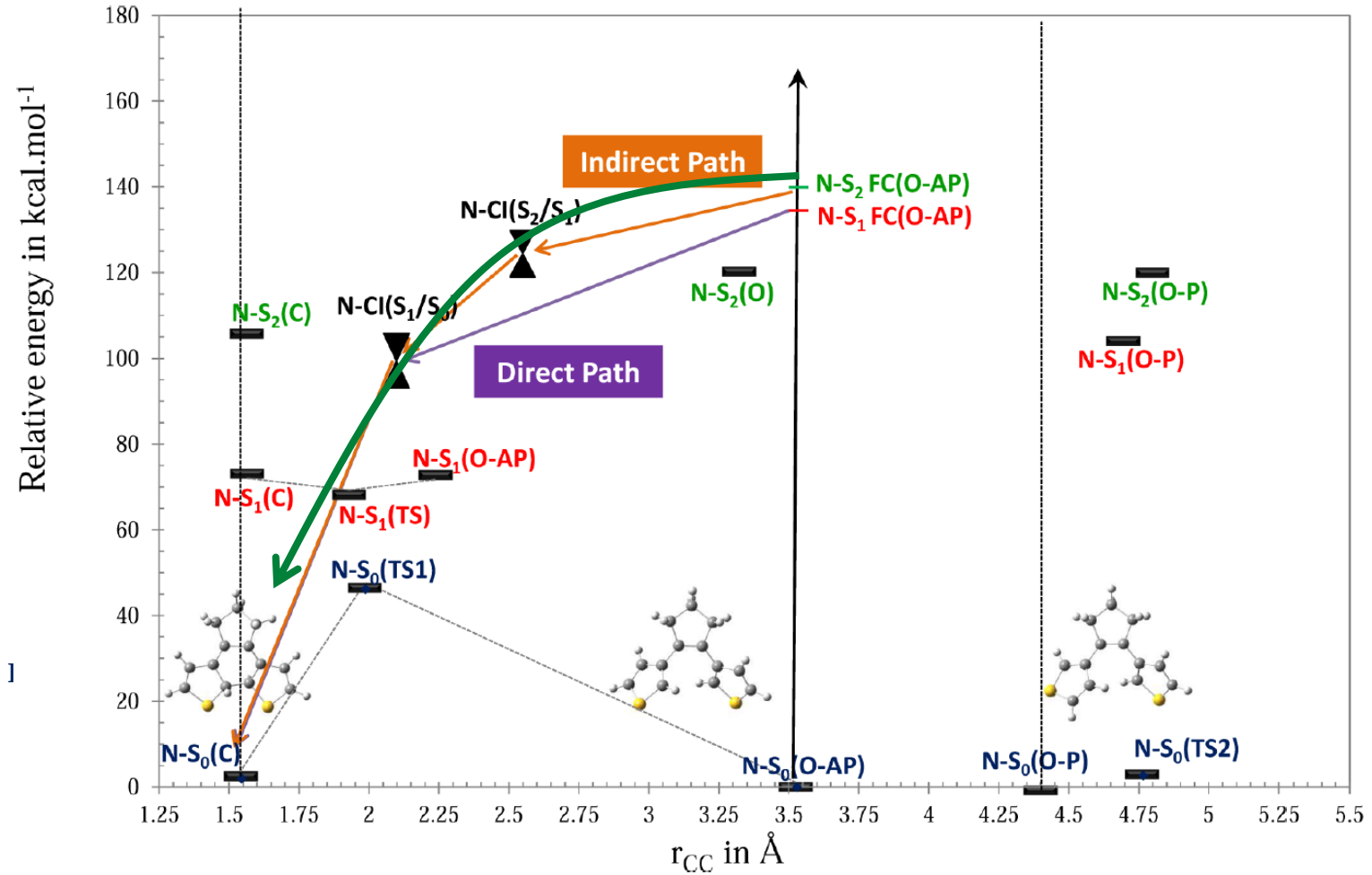


N DTE CASPT2//CASSCF(10,10)/6-31G(d)

Perrier, A.; Aloise, S.; Olivucci, M.; Jacquemin, D. *J. Phys. Chem. Lett. 2013, 4, 2190.*



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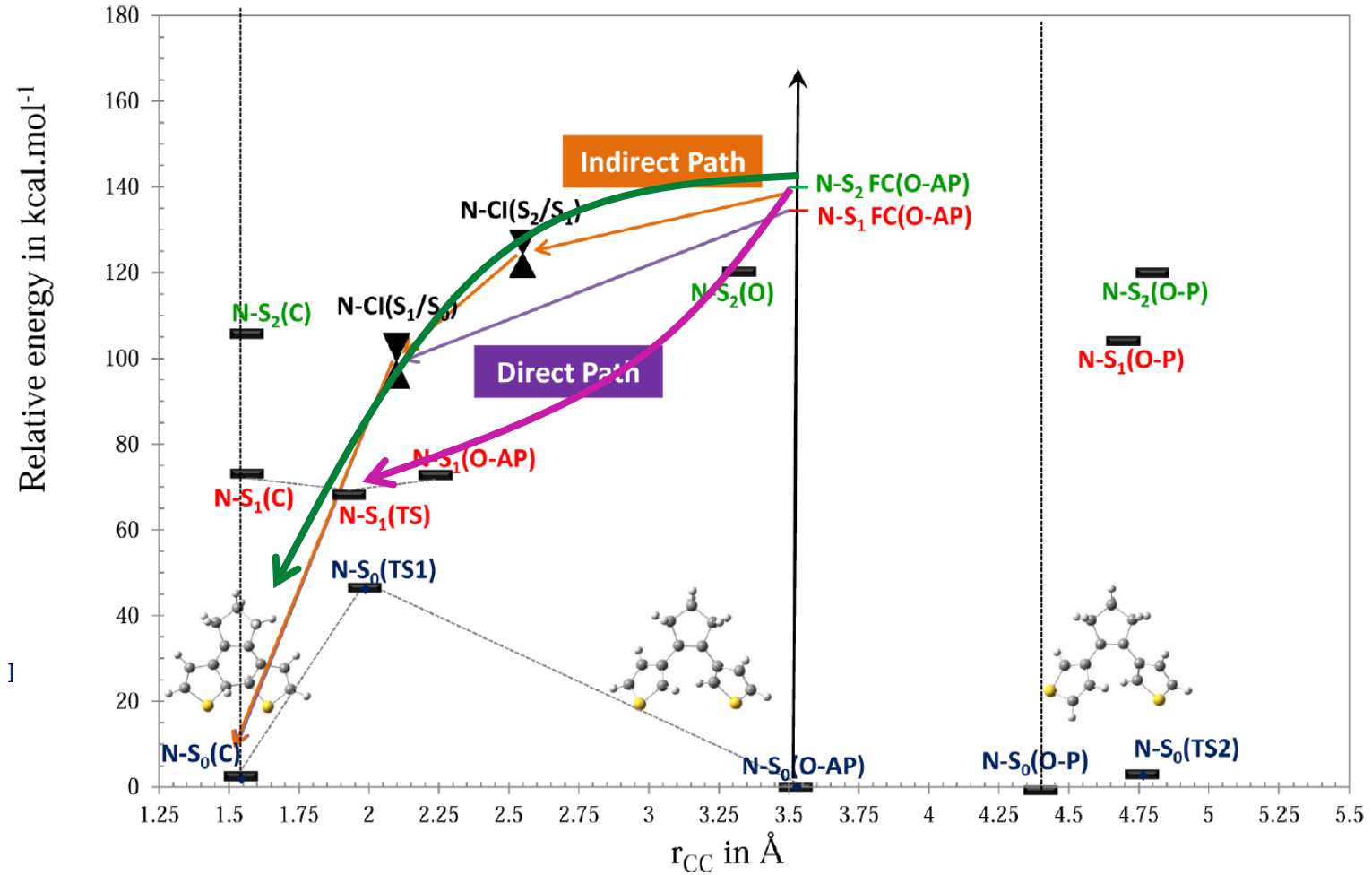

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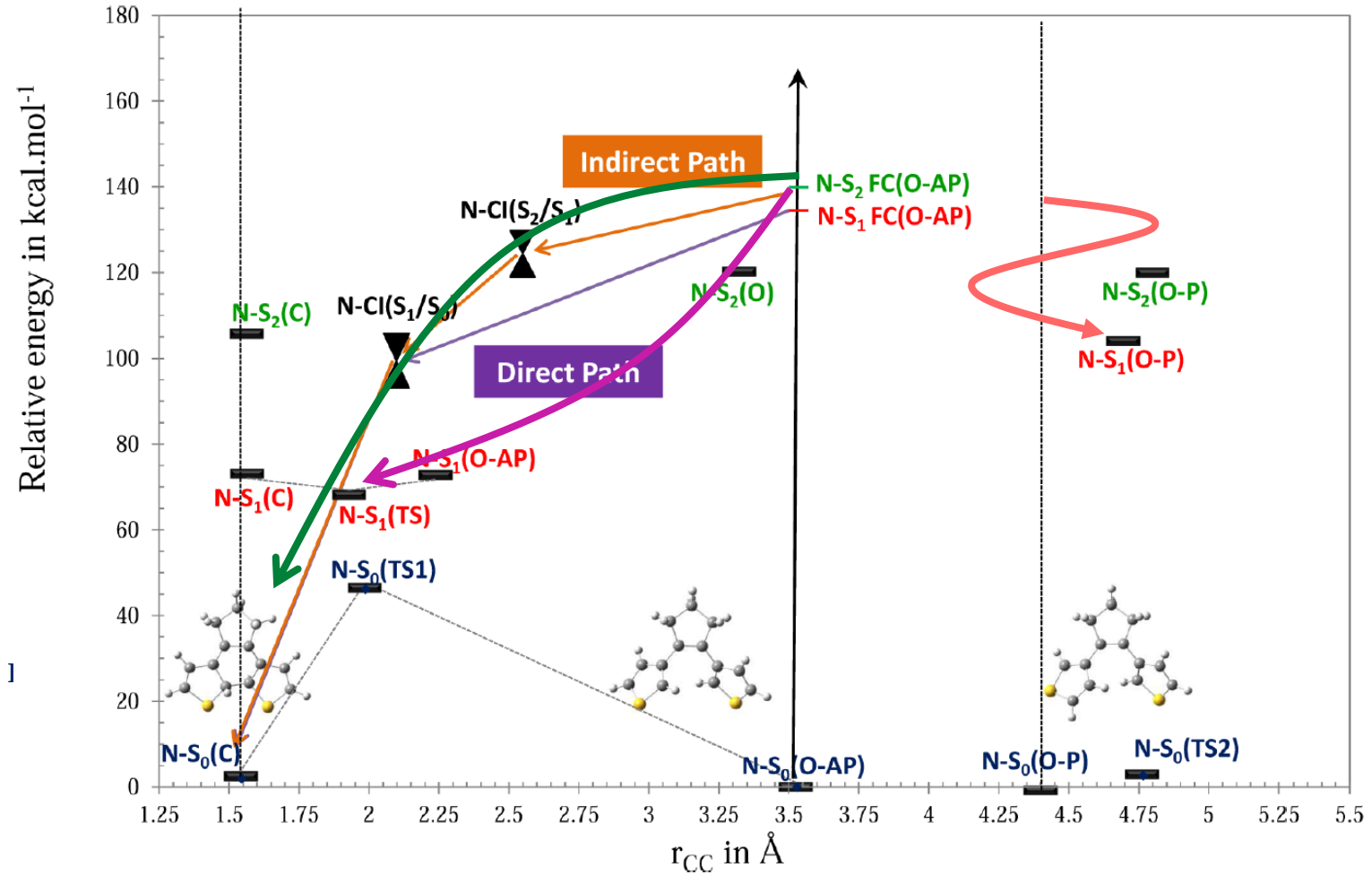

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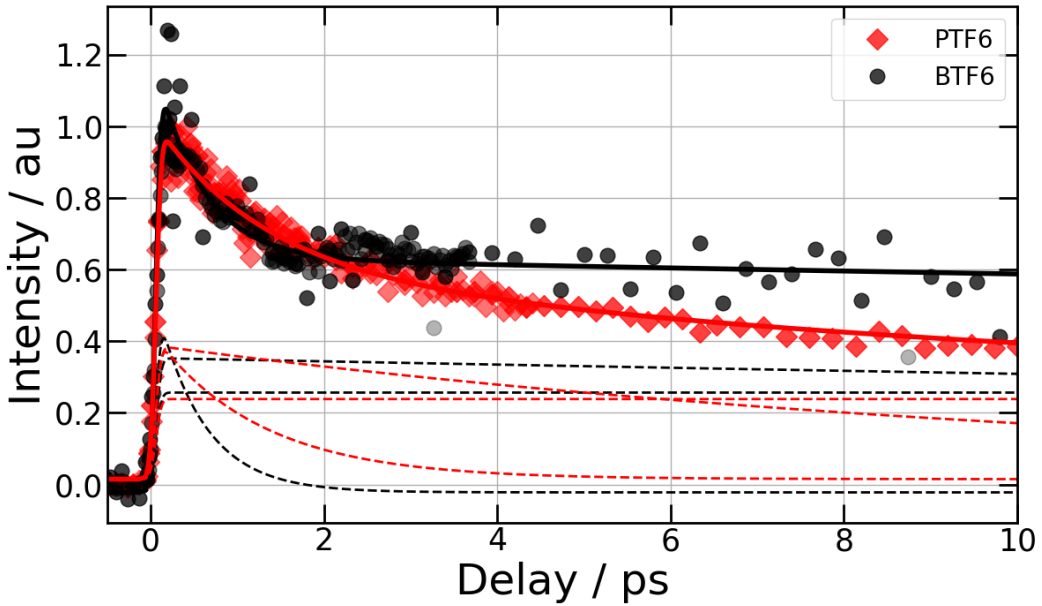
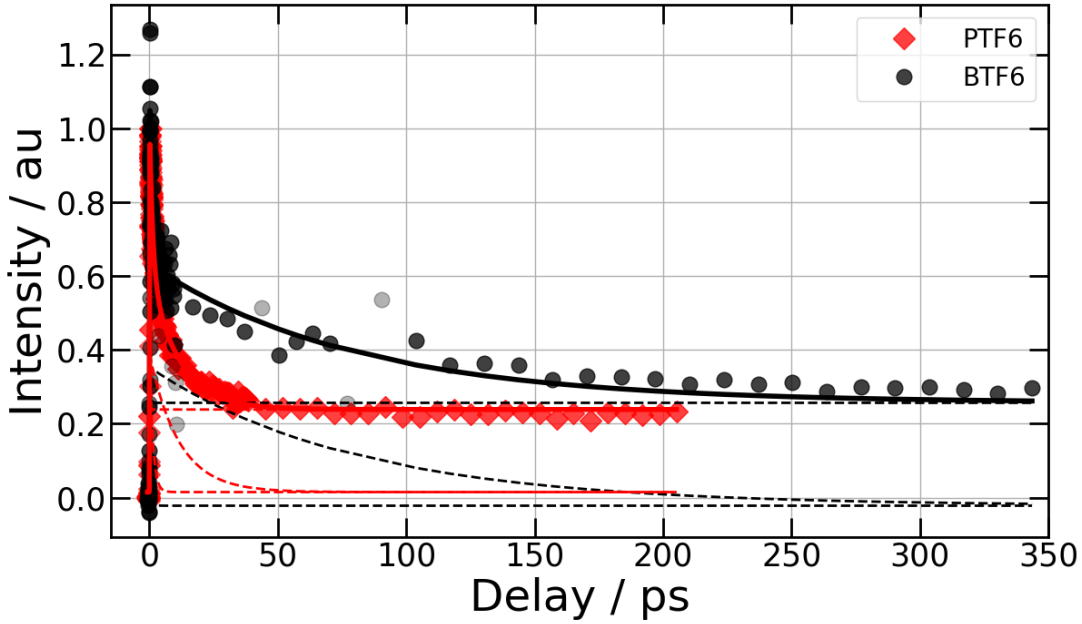
Results on BTF6 and PTF6





BTF6	
0.54 ps	45 %
75 ps	32 %
Plateau	23 %

PTF6	
1.2 ps	40 %
11.4 ps	37 %
Plateau	23 %

Lietard, A.; Piani, G.; Pollet, R.; Soep, B.; Mestdagh, J.-M.; Poisson, L. *Phys. Chem. Chem. Phys. 2022, 24, 9807.*

Effect of the environement

Effect of the environement

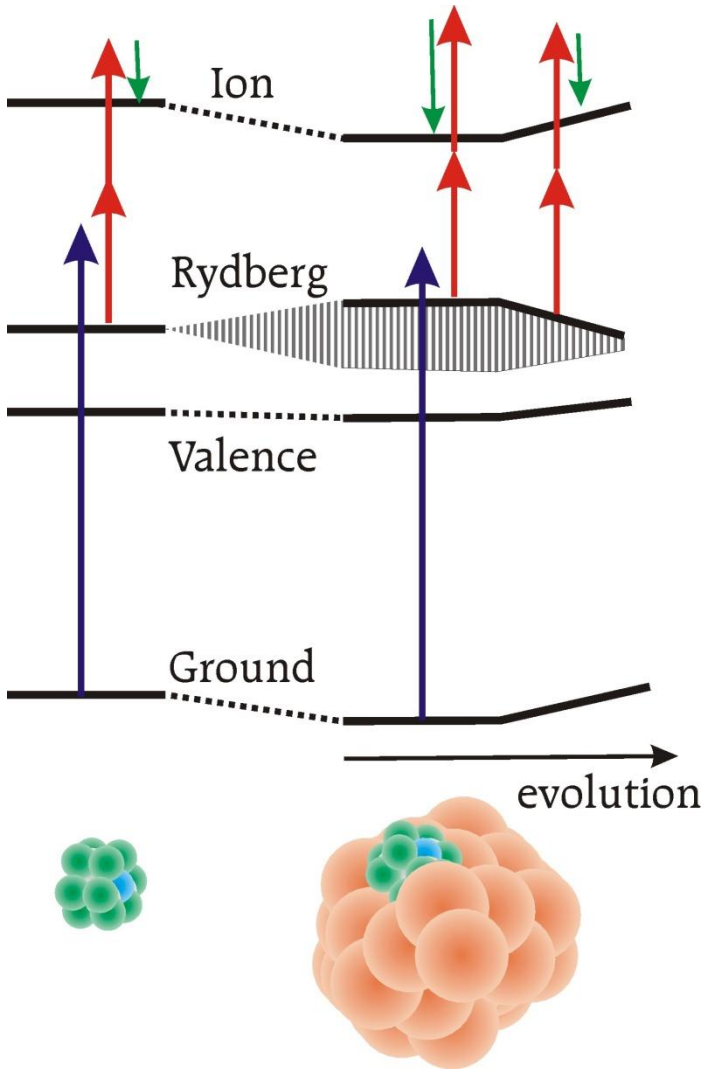
→ Thermalized molecule

Effect of the environement

- Thermalized molecule
- Influence on motion

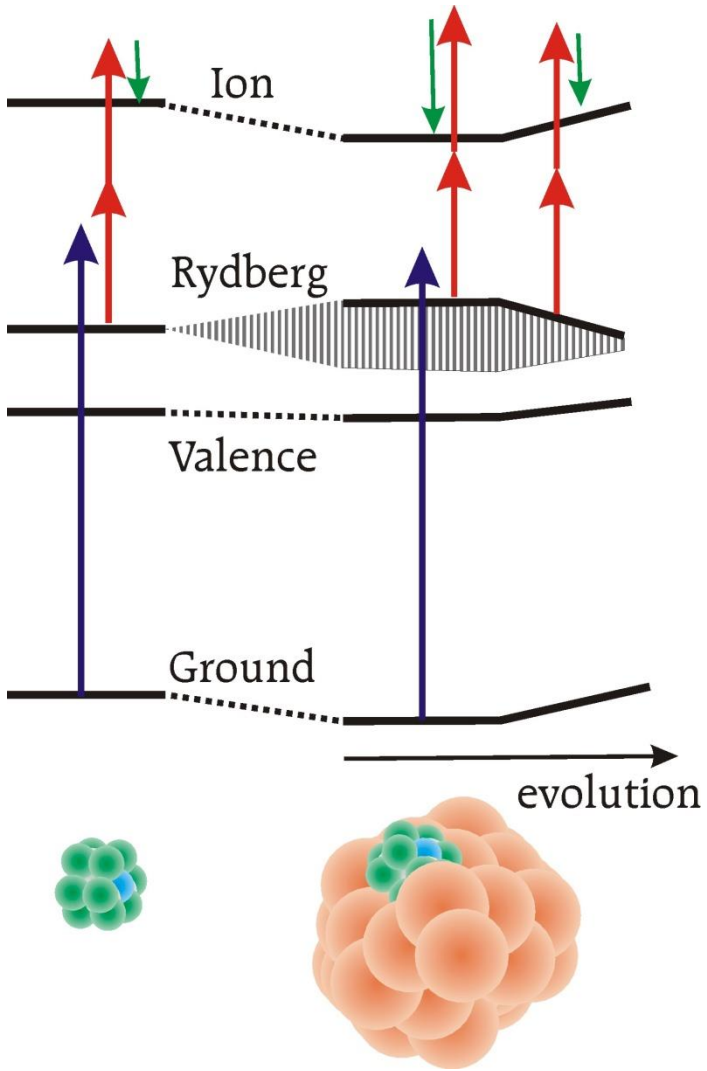
Effect of the environement

- Thermalized molecule
- Influence on motion
- Effects on the electronic states



Effect of the environement

- Thermalized molecule
- Influence on motion
- Effects on the electronic states
- Effect on electron dynamics (conical intersection, symmetry…)



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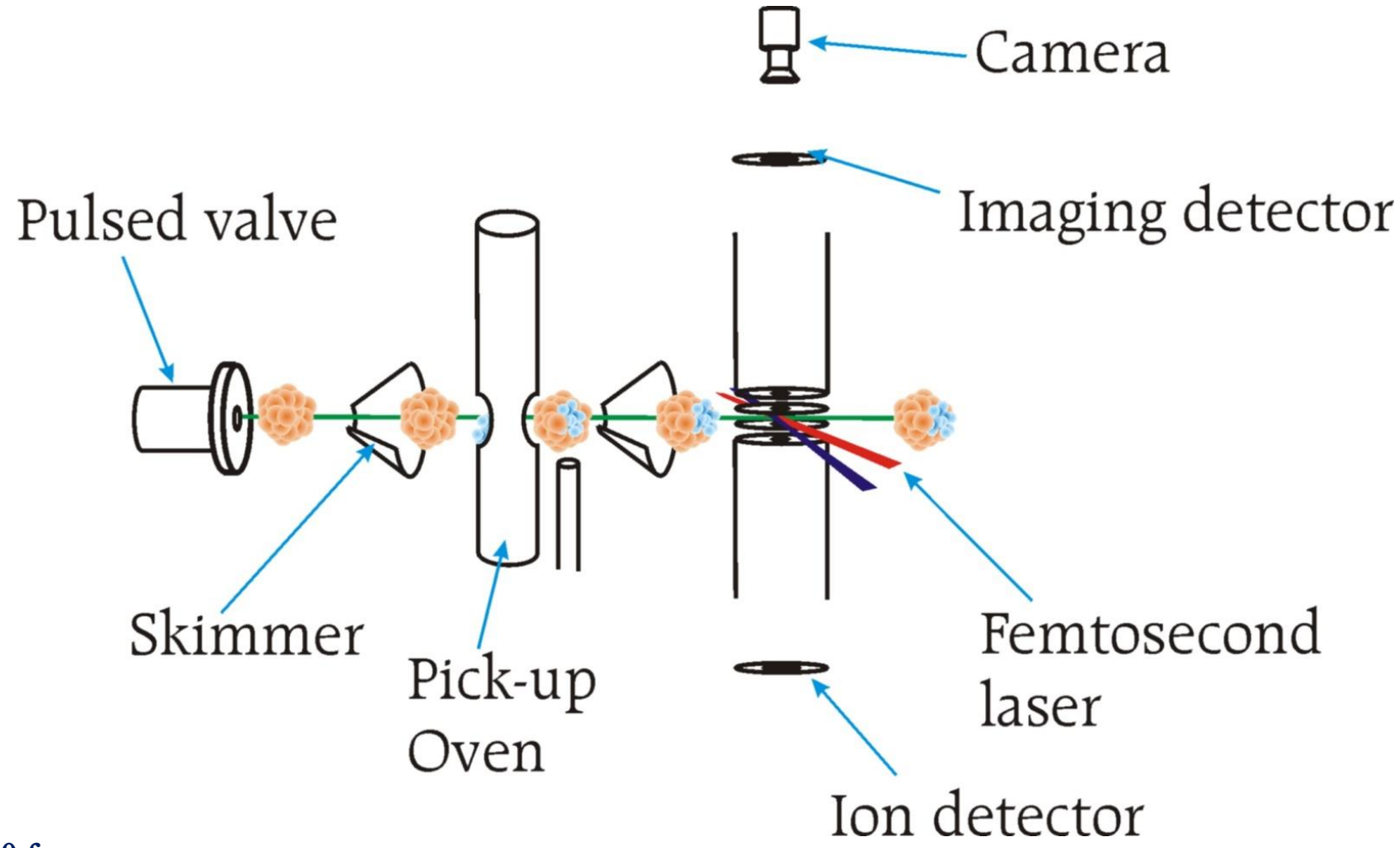

SLIC fs 20 Hz laser facility
800 nm, 2 mJ, 60 fs
266 nm, 200 µJ, 100 fs

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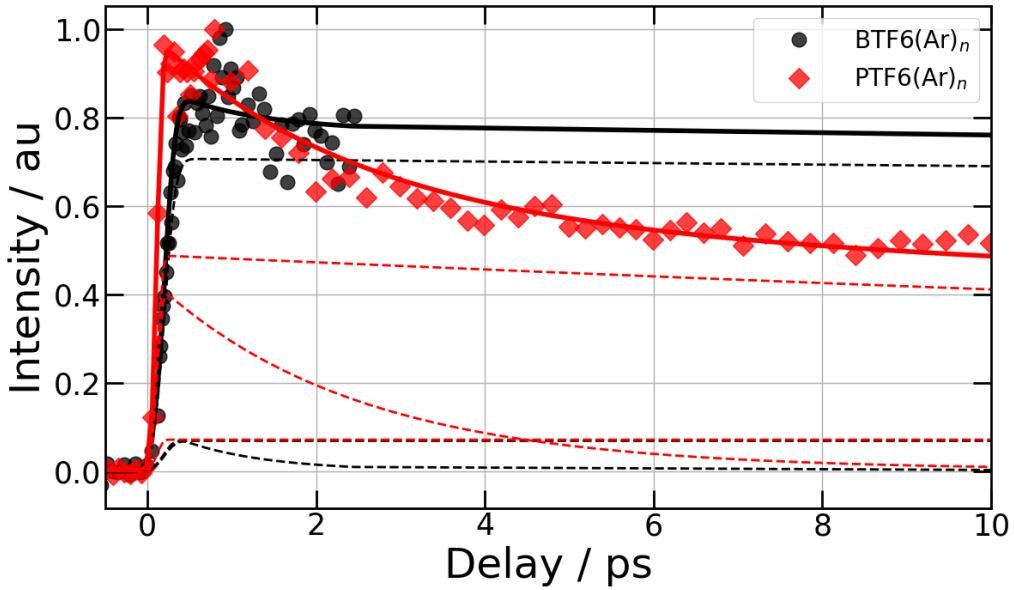
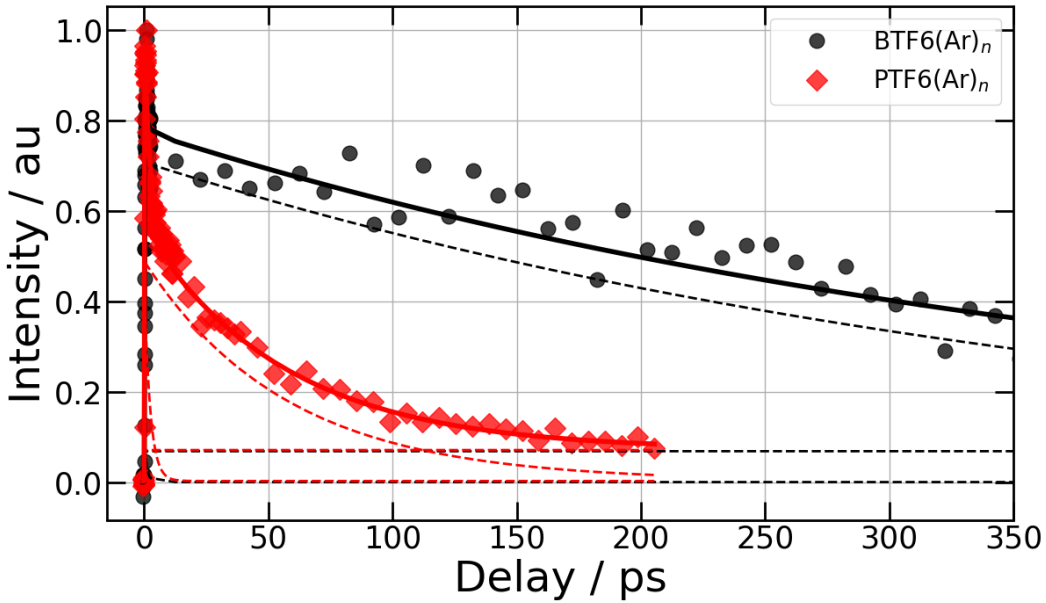
Effect of the environement





BTF6				PTF6			
0.54 ps	45 %	1.0 ps	9 %	1.2 ps	40 %	2.4 ps	43 %
75 ps	32 %	400 ps	82 %	11.4 ps	37 %	57 ps	50 %
Plateau	23 %		8 %	Plateau	23 %		8 %

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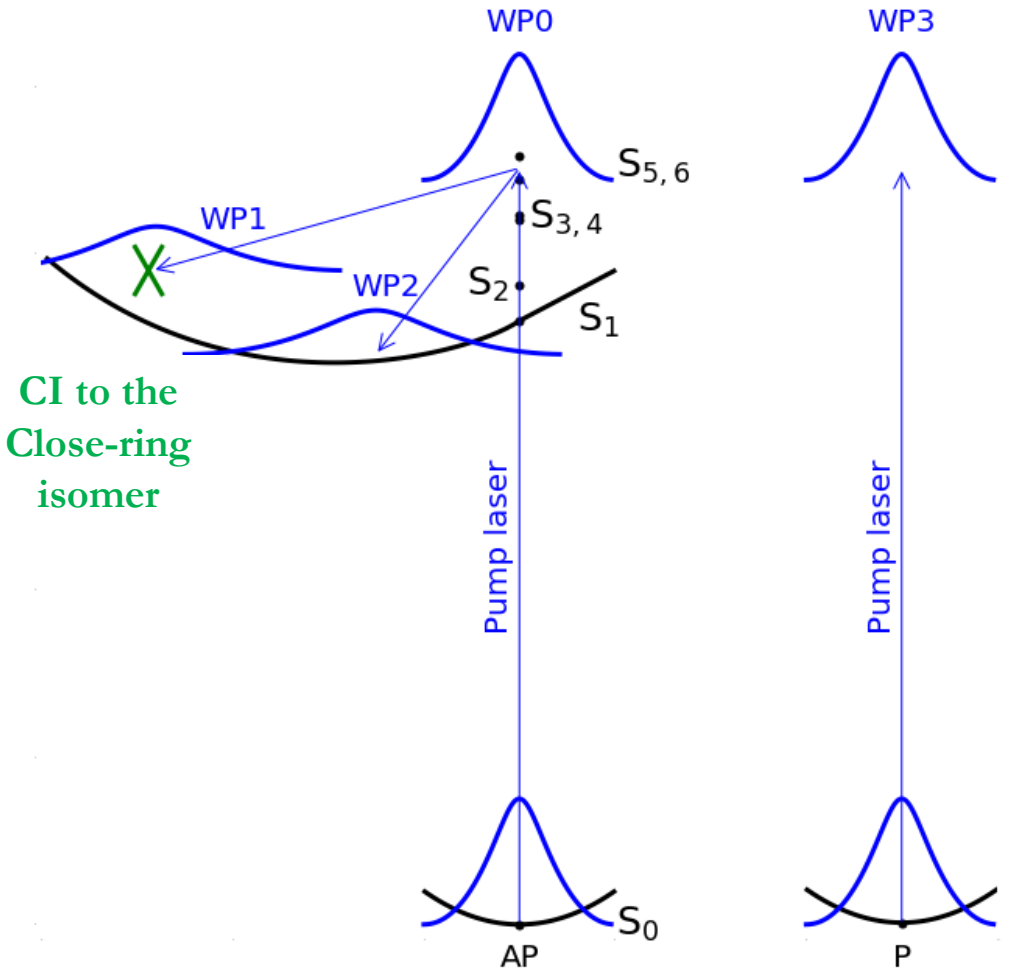
3 WP Model



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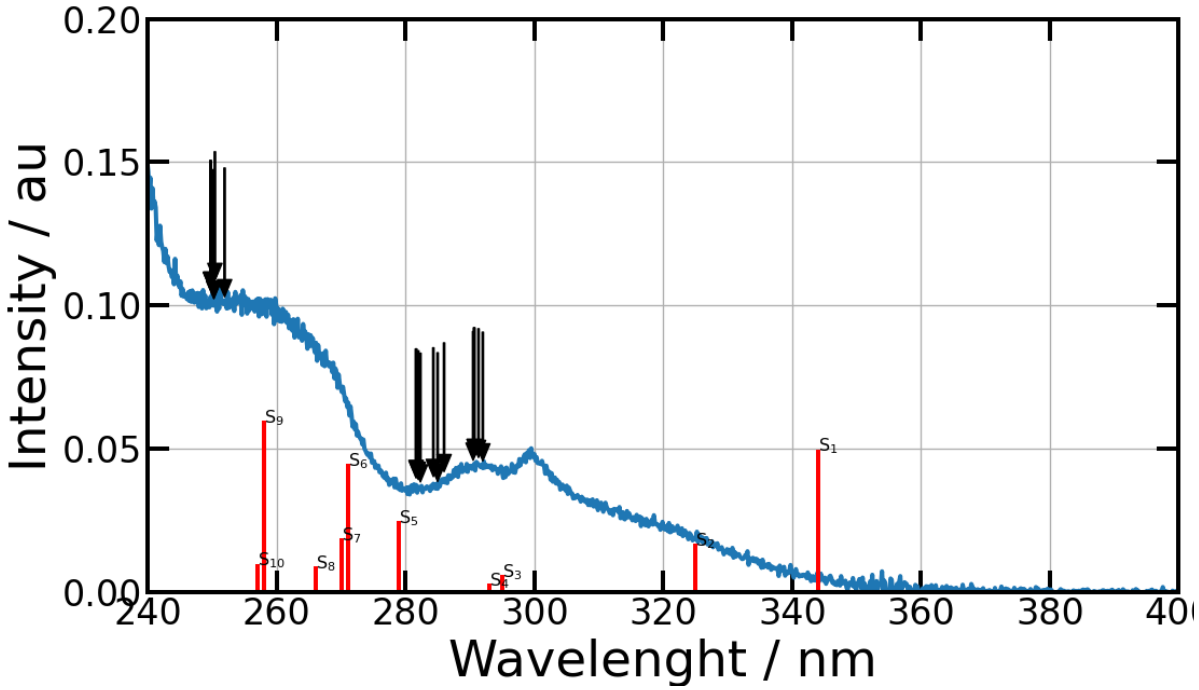
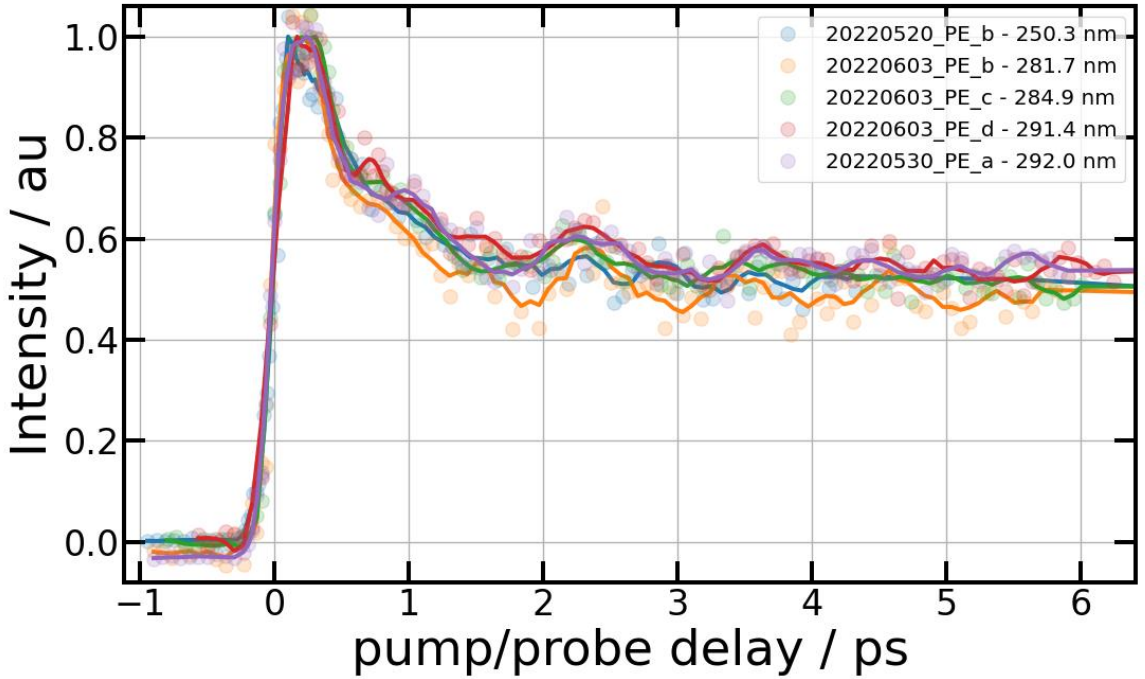
Looking for the conical intersection





Conclusions

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→ Confirmation of the 3 wavepackets model

Conclusions

- Confirmation of the 3 wavepackets model
- Effect on the dynamics of an environment

Conclusions

- Confirmation of the 3 wavepackets model
- Effect on the dynamics of an environment
- Two different pathways, two different reactivities

Aknowledgments

Experimental studies

Cheshta Chopra
Aude Lietard
Giovanni Piani
Lou Barreau
Stéphane Aloïse
Jean-Michel Mestdagh
Benoît Soep

Synthesis

Mashahiro Takeshita — Saga University

Theoretical Support

Rodolphe Pollet — Université Paris-Saclay
Aurélie Perrier — Universite Paris Cité