2D electronic spectroscopy study of TIPS - pentacene

Le, Duc Viet; Leng, Xuan; Do, Thanh Nhut; Tan, Howe Siang; Perrelle, Jessica M. de la; Kee, Tak W.

2020

Le, D. V., Leng, X., Do, T. N., Tan, H. S., Parrelle, J. M. d. l., Kee, T. W. (2020). 2D electronic spectroscopy study of TIPS - pentacene. Proc. Of the 7th Asian Spectroscopy Conference (ASC 2020). doi:10.32655/ASC_8-10_Dec2020.45

<https://hdl.handle.net/10356/144297>

https://doi.org/10.32655/ASC_8-10_Dec2020.45

© 2020 Nanyang Technological University.

Downloaded on 26 Apr 2023 18:02:17 SGT

2D Electronic Spectroscopy study of TIPS - Pentacene

**Duc Viet Le[†], Xuan Leng[†], Thanh Nhut Do[†], Howe Siang Tan[†],
Jessica M. de la Perrelle[‡], Tak W. Kee[‡]**

[†]*School of Physics and Mathematical Science, Nanyang Technological University
21 Nanyang Link, Singapore, 637371*

[‡]*School of Physical Sciences, University of Adelaide, Darling, Adelaide SA 5000, Australia*

E-mail: dvle@ntu.edu.sg

Abstract

The molecule TIPS – Pentacene has gained a lot of attraction recently due to its ability to exhibit the singlet fission phenomenon, which has the potential of improving power conversion efficiency significantly in photovoltaic devices¹. Therefore, investigating into the photophysical properties of this molecule can assist researchers in better understanding the singlet fission phenomenon.

2D Electronic spectroscopy of TIPS – Pentacene in solution shown a strong beating at 265cm⁻¹ in both the amplitude and the central line slope², which corresponds to a breathing mode of the molecule.

Fig 1: (a) Chemical structure of TIPS - Pentacene molecule. (b) 2DES spectrum of the diagonal peak pumped at 645nm and its calculated CLS. (c) The absolute value of the Fourier Transformed map of the diagonal peak along T_w at 265cm⁻¹. (d) Center line slope value as a function of T_w .

The 2D spectra result $S(\omega_1, T_w, \omega_3)$ (Fig. 1a) can be understood using the theory of a two level system coupled to a series of harmonic oscillators³. The resultant lineshape function $g(t)$ of the system can be partitioned into two functions: $g_b(t)$ (environment) and $g_v(t)$ (vibrational mode).

$$g(t) = g_b(t) + g_v(t)$$

A full expansion of the lineshape function $g(t)$ in the third order nonlinear optical response functions can be used to simulate the experimental 2D spectra, including the 2D Fourier map at 265 cm⁻¹ (Fig.1c) and the Centre Line Slope analysis (Fig.1d).

Keyword: two-dimensional spectroscopy, vibrational coherence, center line slope.

References:

- [1] Bakulin, A. A.; Morgan, S. E.; Kehoe, T. B.; Wilson, M. W.; Chin, A. W.; Zigmantas, D.; Egorova, D.; Rao, A., Real-time observation of multiexcitonic states in ultrafast singlet fission using coherent 2D electronic spectroscopy. *Nat Chem* **2016**, 8 (1), 16-23.
- [2] Do, T. N.; Khyasudeen, M. F.; Nowakowski, P. J.; Zhang, Z.; Tan, H.-S., Measuring Ultrafast Spectral Diffusion and Correlation Dynamics by Two-Dimensional Electronic Spectroscopy. *Chemistry – An Asian Journal* **2019**, 14 (22), 3992-4000.
- [3] Mukamel, S., *Principles of nonlinear optical spectroscopy*. 1995.