

## Introducing position effect of trifluoromethyl moiety on bis-styrylbenzene skeleton

Hiroyuki Mochizuki

Research center for photovoltaics  
National Institute of Advanced Industrial Science and Technology  
1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan  
Phone: +81-29-861-5034 E-mail: h-mochizuki@aist.go.jp

### Abstract

**5 kinds of bis-styrylbenzene derivatives with trifluoromethyl moieties were prepared, and their properties were also evaluated. The characteristics of bis-styrylbenzene derivatives changed remarkably depending introduction position. In the present study, the compounds with the higher molecular weight did not always show the higher melting point.**

### 1. Introduction

Of the organic functional skeletons, bis-styrylbenzene derivatives are promising in terms of showing high emission abilities and electron mobilities [1-4]. Introduction effects of substituents on organic compounds are effective for change in the characteristics, such as change in the melting point, the crystallinity, the surface energy, the miscibility, and the ionizing potential, etc [5-7]. There was report on the bis-styrylbenzene derivatives substituted with methyl moieties, and their characteristics were altered by the introduction position of methyl moieties [7]. Among the substituents, trifluoromethyl moiety is of interest to change markedly ionizing potential values. As the variation in ionizing potential controls the electronic carrier type, there have been many reports on electronic properties of organic functional compounds with trifluoromethyl moieties [9-12].

I reported the photo-physical properties of 1,4-bis(2-trifluoromethylstyryl)benzene in detail [13]. Here, I also report the effect of introduction position for trifluoromethyl moiety on the properties of bis-styrylbenzene derivatives.

### 2. Experiment

I synthesized 5 kinds of bis-styrylbenzene derivatives with trifluoromethyl moieties by the Horner-Wadsworth-Emmons (HWE) reaction reported previously [14-17]: the prepared compound were 1,4-bis(2-trifluoromethylstyryl)benzene (2CF3), 1,4-bis(3-trifluoromethylstyryl)benzene (3CF3), 1,4-bis(4-trifluoromethylstyryl)benzene (4CF3), 1,4-bis(3,5-difluoromethylstyryl)benzene (d3,5CF3), and 1,4-bis(2,4-difluoromethylstyryl)benzene (d2,4CF3). The HWE reaction allowed the product through only re-crystallization.

### 3. Results and discussion

The chemical structures and the melting points (MPs) of the prepared compounds were summarized in Table 1. All the bis-styrylbenzene derivatives were obtained with the yield

range from 70 to 90%.

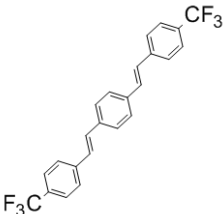
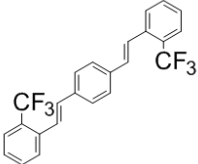
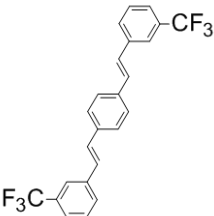
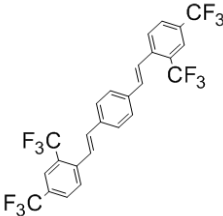
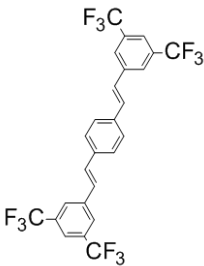
Molecular weights of bis-styrylbenzene derivatives substituted with 2 trifluoromethyl moieties and 4 trifluoromethyl moieties were 434 and 554, respectively. Among the compounds with the molecular weight of 434, 4CF3 showed the highest MP of 273°C. The MPs of 2CF3 and 3CF3 were 133°C and 144°C, respectively, which were lower than that of 4CF3. The MP of d3,5CF3, which showed a good molecular symmetry and had the higher molecular weight than 4CF3, was 197°C. It was lower than that of 4CF3. In the present study, the compounds with the higher molecular weight did not always show the higher MP.

All the compound prepared in the present study strongly emitted fluorescence at a blue region.

### References

- [1] Z. Yang, H. J. Geise, M. Mehbod, G. Debrue, J. W. Visser, E. J. Sonneveld, L. Van't dack and R. Gijbels, *Synth. Met.* **39** (1990) 137.
- [2] C. C. Wu, M. C. DeLong, Z. V. Vardeny, J. P. Ferraris and J. J. Gutierrez, *Synth. Met.* **137** (2003) 939.
- [3] H. Wang, F. Li, B. Gao, Z. Xie, S. Liu, C. Wang, D. Hu, F. Shen, Y. Xu, H. Shang, Q. Chen, Y. Ma, and H. Sun, *Cryst. Growth Des.* **9** (2009) 4945.
- [4] J. Gierschner and S. Y. Park, *J. Mater. Chem. C*, **1** (2013) 5818.
- [5] U. Stalmach, D. Schollmeyer, and H. Meier, *Chem. Mater.* **11** (1999) 2103.
- [6] M. L. Renak, G. P. Bartholomew, S. Wang, P. J. Ricatto, R. J. Lachicotte, and G. C. Bazan, *J. Am. Chem. Soc.*, **121** (1999) 7787.
- [7] R. Kabe, H. Nakanotani, T. Sakanoue, M. Yahiro, and C. Adachi, *Adv. Mater.* **21** (2009) 4034.
- [8] T. Yasuda, M. Saito, H. Nakamura, and T. Tsutsui, *Appl. Phys. Lett.* **89** (2006) 182108.
- [9] S. Hotta and T. Yamao, *J. Mater. Chem.* **21** (2011) 1295.
- [10] S. K. Park, J. H. Kim, S.-J. Yoon, O. K. Kwon, B.-K. An, and S. Y. Park, *Chem. Mater.* **24** (2012) 3263.
- [11] S. K. Park, S. Varghese, J. H. Kim, S.-J. Yoon, O. K. Kwon, B.-K. An, J. Gierschner, and S. Y. Park, *J. Am. Chem. Soc.* **135** (2013) 4757.
- [12] H. Nakanotani and C. Adachi, *Appl. Phys. Lett.* **96** (2010) 053301.
- [13] H. Mochizuki, Y. Sonoda, F. Sasaki, and R. Azumi, *Jpn. J. Appl. Phys.* **55** (2016) 022101.
- [14] B. E. Maryanoff and A. B. Reitz, *Chem. Rev.* **89** (1989) 863.
- [15] K. Sato, M. Higuchi, N. Iwata, T. C. Saido, and K. Sasamoto, *Eur. J. Med. Chem.* **39** (2004) 573.
- [16] D. P. Flaherty, S. M. Walsh, T. Kiyota, Y. Dong, T. Ikezu, and J. L. Vannerstrom, *J. Med. Chem.* **50** (2007) 4986.
- [17] I. Kikaš, B. Carlotti, I. Škorić, M. Šindler-Kulyka, U. Mazucato, and A. Spalletti, *J. Photoch. Photobio. A* **244** (2012) 38.

Table I The chemical structures and the melting point of prepared in the present study.

| Abbreviated name   | 4CF3                                                                              | 2CF3                                                                              | 3CF3                                                                              | d2,4CF3                                                                             | d3,5CF3                                                                             |
|--------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| Chemical structure |  |  |  |  |  |
| Melting point      | 274°C                                                                             | 133°C                                                                             | 144°C                                                                             | 230°C                                                                               | 197°C                                                                               |