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Characteristics of bis-styrylbenzene derivatives with various electron-withdrawing groups

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Abstract

We synthesized 5 kinds of bis-styrylbenzene derivatives with various electron-withdrawing groups by the Horner-Wadsworth-Emmons reaction. The introduced electron-withdrawing groups were trifluoromethyl, trifluoromethyloxy, trifluoromethylthio, cyano, and nitro moieties. The substituted position was both terminals of bis-styrylbenzene. The cyano moiety had a great effect on increase in the melting point of bis-styrylbenzene derivatives.

1. Introduction

Bis-styrylbenzene derivatives show high photo-physical and electronic properties due to their molecules conjugated extensively [1-3]. Their molecular planarity also allows good crystallinity, high melting point and high sublimation [4]. As characteristics of bis-styrylbenzene change markedly depending of substituent introduction, there have been reports on the bis-styrylbenzene derivatives with various substituents [5,6].

Trifluoromethyl moieties have been of interest because it is effective for improvement in the characteristics, such as increase in the electron-withdrawing ability, rise in the hydrophobicity, reduction in the melting point, etc [7-10]. We have evaluated photo-physical properties of 1,4-bis(4-trifluoromethylstyryl)benzene in detail, however, the effect of trifluoromethyl moiety on the photo-physical properties of bis-styrylbenzene was similar to that of methyl moiety [11].

Here, we report the introduction effects of various electron-withdrawing groups on properties of the bis-styrylbenzene derivatives.

2. Experiment

5 kinds of bis-styrylbenzene derivatives were synthesized by the Horner-Wadsworth-Emmons (HWE) reaction reported previously [2,12-15]. A 28 % methanol solution of sodium methoxide was added dropwise to a stirred mixture of *p*-bis(diethylphosphono)xylene and benzaldehyde with various electron-withdrawing groups in *N*,*N*-dimethylformamide (DMF) at rt. This mixture was then heated to 80 °C for 2 h. The reaction was then quenched with 2:1 DMF/H_2O and recrystallized from toluene affording the desired compounds: 1,4-bis(4-trifluoromethylstyryl)benzene (4CF3), 1,4-bis(4-trifluoromethyloxystyryl)benzene (4OCF3), 1,4-bis(4-trifluoromethylthiostyryl)benzene (4SCF3), 1,4-bis(4-cyanostyryl)benzene (4CN), 1,4-bis(4-nitrostyryl)benzene (4NO2).

3. Results and discussion

The chemical structures and melting points of the prepared compounds are summarized in Table 1. Among the prepared 5 compounds, the melting points of 4CN was highest of 286˚C, even its molecular weight was lowest of 332. On the other hand, the melting point of 4SCF3 having the highest molecular weight was the lowest of 182˚C. The cyano moiety promoted the molecular stacking leading to high melting points.

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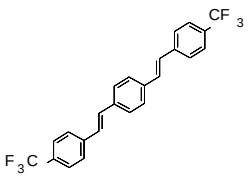
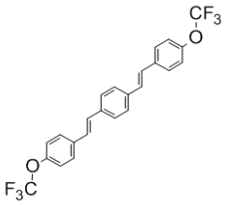
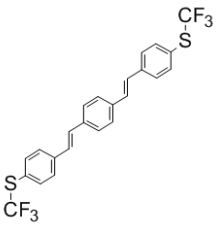
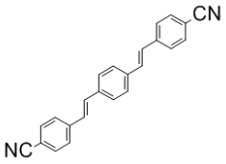
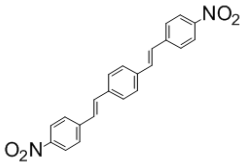
Table I The chemical structures and the melting point of prepared in the present study.

Abbrevi-ated name	**4CF3**	**4OCF3**	**4SCF3**	**4CN**	**4NO2**
Chemical structure					
Melting point	274°C	242°C	182°C	286°C	286°C