テトラキス(メチルカルコゲノ)ジセレナシクロペンタフルオレンの合成と結晶構造

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Synthesis and crystal structures of tetrakis(methylchalcogeno)diselenacyclopentafluorenes

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Recently, we have reported that tetrakis(methylthio)pyrene exhibited very high carrier mobility exceeding 30 cm^2 / V s (Fig. 1a).[1)] To enhance further mobility, we designed selenium-containing isoelectronic compounds, namely tetrakis(methylchalcogeno)diselena-cyclopentafluorenes (**1** and **2**, Fig. 1a), focusing on their small reorganization energies and their potential for promoting intermolecular orbital interactions in the solid state. From parent diselenacyclopentafluorene (**3**),[2)] the preparation of which was accomplished by a newly developed two-step method (33%, Fig. 1b), compounds **1** and **2** were synthesized by regio-selective bromination followed by the introduction of methylchalcogeno groups. We also elucidated the crystal structures of **1** and **2** by single-crystal X-ray analysis. In the presentation, we will discuss the correlation between the crystal structures and carrier transport properties of **1** and **2**.

Keywords : chalcogen atom; crystal structure; organic semiconductor; methylchalcogeno group

最近我々は、テトラキス (メチルチオ) ピレンが 30 cm^2/Vs を超える非常に高い移動度を示すことを報告した[1)]。本研究ではさらなる移動度の向上を図るため、固体中での軌道相互作用の促進が可能で、再配向エネルギーが小さいことに着目し、セレンを含む等電子化合物、テトラキス (メチルカルコゲノ) ジセレナシクロペンタフルオレン (**1**, **2**, Fig. 1a) を設計した。新たに開発した効率的な合成法 (33%/2 steps, Fig. 1b) により無置換体 **3**[2)] を得た後、**3** の位置選択的な臭素化とメチルカルコゲノ基の導入により **1**、**2** を合成した。また、単結晶 X 線構造解析により **1**、**2** の結晶構造を明らかにしており、発表では、**1**、**2** の結晶構造と電荷輸送特性との相関について報告する予定である。

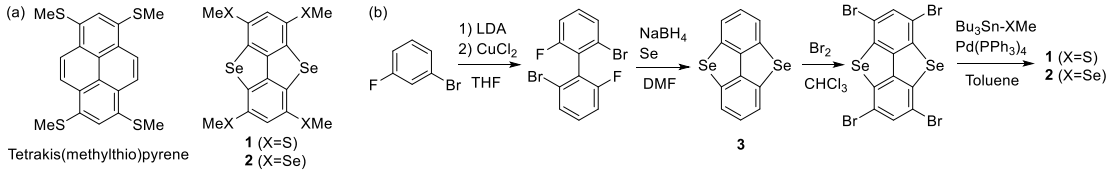

Fig. 1. (a) Chemical structures of tetrakis(methylthio)pyrene and the selenium-containing isoelectronic analogues **1** and **2** and (b) the synthetic route to the analogues.

1) K. Takimiya, et al., *Adv. Mater*. **2021**, *33*, 2102914.
2) T. kimura, et al., *Heterocycles* **1994**, *37*, 541-552.