分子末端にフッ素原子を導入した[5]および[6]フェナセンの合成と電子スペクトル

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Synthesis and spectral properties of phenacenes fluorinated at the edges of the molecule ([1]*Graduate School of Environment, Life, Natural Science and Technology, Okayama University*, [2]*Graduate School of Science and Technology, Gunma University*, [3]*Institute for Materials Chemistry and Engineering, Kyushu University*, [4]*Faculty of Environment, Life, Natural Science and Technology, Okayama University*) ○Yuuki Ishii,[1] Minoru Yamaji,[2] Fumito Tani,[3] Kenta Goto,[3] Hideki Okamoto[1,4]

It has been noted that structural and electronic features of polycyclic aromatic hydrocarbons are modified by fluorination on the aromatic cores. In this work, influence of fluorine atoms on electronic properties of phenacenes have been investigated. Thus, octafluorofulminene (**F8FUL**) and octafluoropicene (**F8PIC**) were synthesized and their electronic spectra were measured. Fluorescence spectrum of **F8FUL** in solution showed clear vibrational structures (Fig. 1a) and red shifted by 5 nm compared to that of the parent compound **FUL**. In contrast, in the solid state, **F8FUL** showed broad and red shifted fluorescence band in a 400-650 nm region (Fig. 1b) suggesting that the solid state structural and electronic features were affected by the fluorination.
Keywords : phenacene, PAH, fluorine

フッ素原子が多環芳香族化合物の電子特性や結晶構造に影響をおよぼすことが報告されてきた．本研究では，フッ素原子がフェナセンの電子スペクトルにおよぼす影響を明らかにすることを目的として，フェナセン骨格にフッ素原子を導入したフッ素化フルミネン（**F8FUL**）およびピセン（**F8PIC**）を合成し電子スペクトルを観測した．溶液中では **F8FUL** の蛍光スペクトルは振動構造を維持し，母体[6]フェナセンと比較して 5 nm 長波長へシフトした (Fig. 1a)．固体中においては **F8FUL** の蛍光スペクトルは母体化合物に比べて顕著にブロード化した (Fig. 1b)．このことから，フッ素置換によって電子特性と固体構造が影響を受けることが示唆される．フッ素化ピセン（**F8PIC**）の電子スペクトル挙動についても報告する．

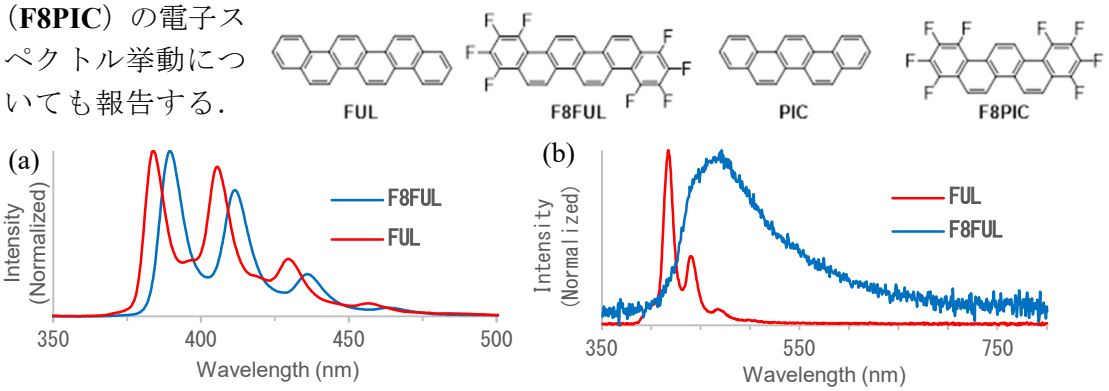

Figure 1. Fluorescence spectra of **FUL** and **F8FUL** in $CHCl_3$ (a) and solid state (b).