

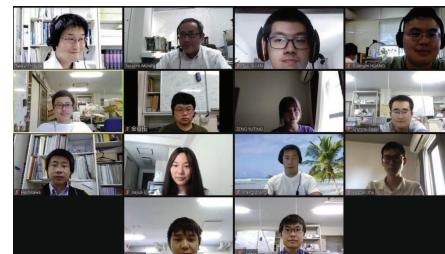
■構造有機化学領域の最近の研究

物質創製化学研究系 構造有機化学研究室

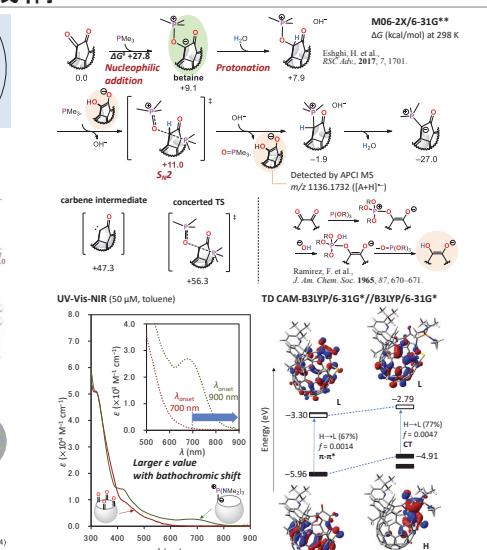
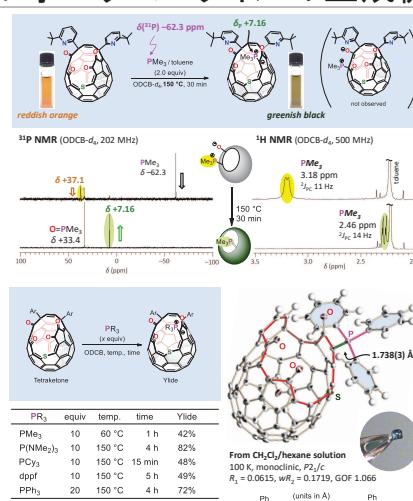
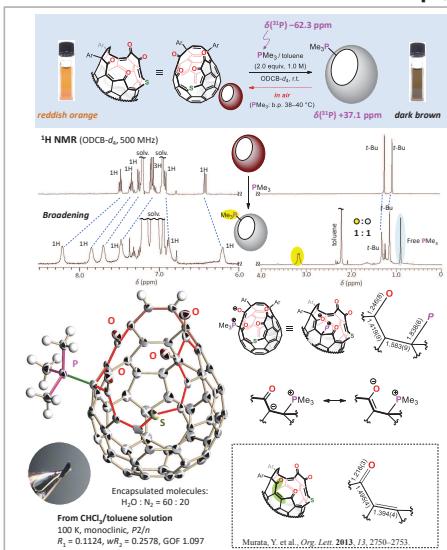
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1. フラーレン誘導体の開口部を反応場としたホスフォニウムベタインの生成機構



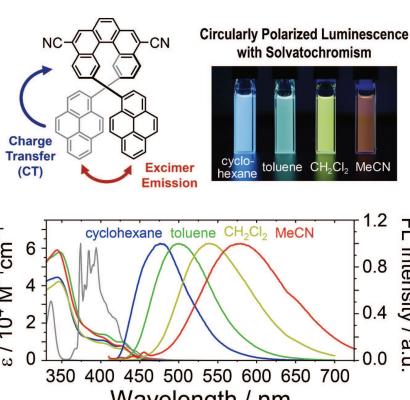
2. らせん状に空間配置したビレンダイマーの発光特性評価

Hirose, T.; Koyama, T.; Hashikawa, Y.; Murata, Y. *manuscript in preparation.*

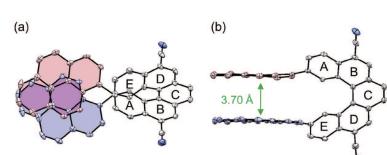
Pyrenes as a Unique FL-Dye:

Table 1. Luminescence properties of general π -conjugated dyes.			
$\Phi_f = 0.21$	$\Phi_f = 0.36$	$\Phi_f = 0.72$	$\Phi_f = 0.71$
$T_F / \text{ns} = 105$	$T_F / \text{ns} = 4.9$	$T_F / \text{ns} = 530$	$T_F / \text{ns} = 4.1$
$k_f / \text{ns}^{-1} = 0.002$	$k_f / \text{ns}^{-1} = 0.07$	$k_f / \text{ns}^{-1} = 0.0014$	$k_f / \text{ns}^{-1} = 0.17$
$K_{\text{ff}} / \text{ns}^{-1} = 0.008$	$K_{\text{ff}} / \text{ns}^{-1} = 0.13$	$K_{\text{ff}} / \text{ns}^{-1} = 0.0005$	$K_{\text{ff}} / \text{ns}^{-1} = 0.07$

Solvatochromism of Emission:



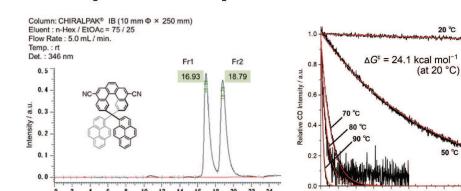
X-ray Crystal Structure:



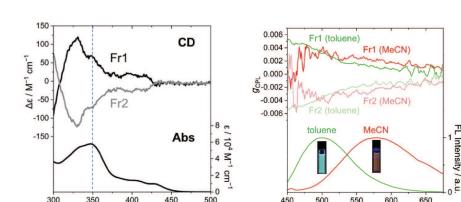
Recorded at 100 K; Space group, Cc; $a = 30.810(12)$ Å; $b = 8.212(3)$ Å; $c = 31.179(12)$ Å; $\beta = 97.57(16)$; $V = 78025(2)$ Å 3 . Data/restraints/parameter = 13765/2/1099; Goodness-of-fit on $R^2 = 1.069$, $R_1 = 0.0432$, $wR_2 = 0.1233$.

✓ Blue-to-orange emission color change depending on solvent polarity.

Chiroptical Properties:



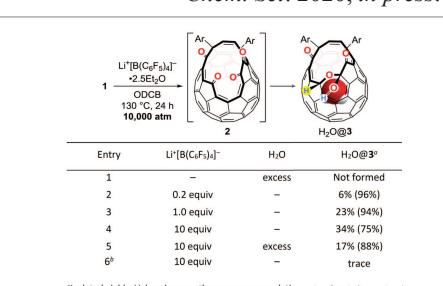
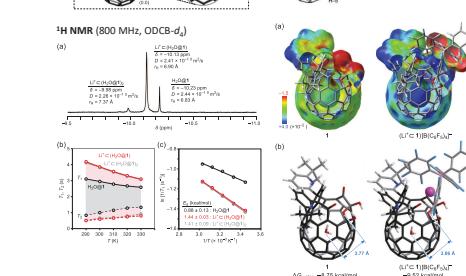
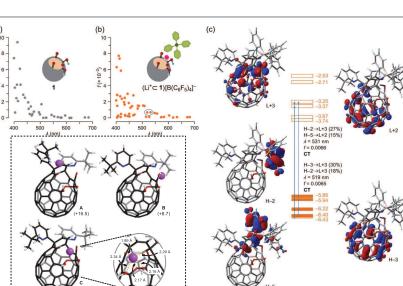
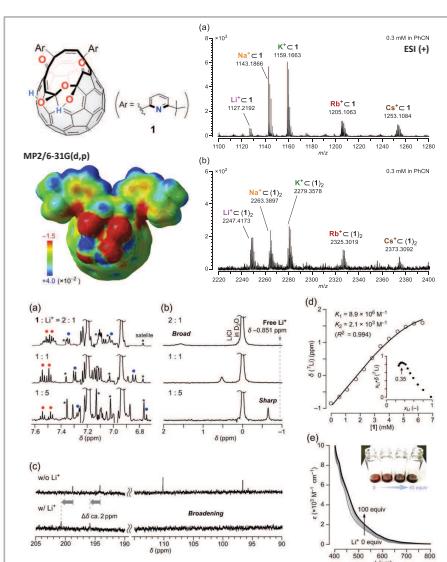
✓ A dynamic helical inversion upon heating.



✓ $\Phi_f = 70\%$, $|g_{\text{lum}}| = 3.2 \times 10^{-3}$ in toluene.

3. 開口フラーレン誘導体を用いたアルカリ金属イオンとの錯形成

Hashikawa, Y.; Murata, Y. *Chem. Sci. 2020, in press.*



^aIsolated yields. Values in parentheses are encapsulation ratio of H₂O determined by ¹H NMR. ^bConducted under ambient pressure.

