Mechanochromic Luminescence of Anthracene-Based *ortho*-Carborane Derivatives

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Mechanochromic Luminescence (MCL) is the reversible luminescent color change induced by mechanical stimuli in the solid-state.[1] We recently reported various stimuli-responsive molecules based on an icosahedral boron and carbon cluster, *ortho*-Carborane (Figure 1, CB),[2] which has a spherical shape and a few intermolecular interaction sites. Due to these unique characteristics, CB can rotate in the crystalline states and form fragile packings. Therefore, CB can be a versatile platform for constructing solid-state stimuli-responsive molecules.[3]

In this work, we synthesized 1,8-bis-*ortho*-Carboranyl anthracene derivatives **1** and **2** (Figure 2). It was revealed that **1** has two types of crystal polymorphs and both **1** and **2** have MCL. When **1** was recrystallized from CCl_4, yellow-emissive crystal (crystal α) was formed and when **1** was recrystallized form common solvents such as $CHCl_3$ and toluene, orange-emissive crystal (crystal β) was formed. Crystal α changes its emission color from yellow to orange upon mechanical grinding (Figure 2). Interestingly, **2**, which has ethynylene spacers between CB and anthracene units exhibited the opposite directional MCL. That is, luminescent color of crystalline **2** is changed from orange to yellow green by mechanical grinding (Figure 2).

In our presentation, we will discuss about detailed properties and plausible mechanism of polymorphs and MCL.

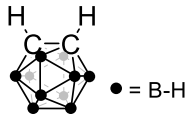

Figure 1. Chemical structure of CB.

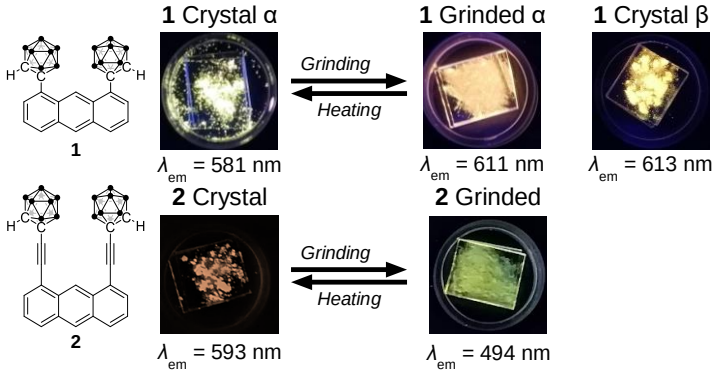

Figure 2. Chemical structures and MCL behaviors of **1** and **2**.

1) S. Ito, *Chem. Lett.* **2021**, *50*, 649–660. 2) a) H. Naito, Y. Morisaki, Y. Chujo, *Angew Chem. Int. Ed.* **2015**, *54*, 5084–5087. b) H. Mori, K. Nishino, K. Wada, Y. Morisaki, K. Tanaka, Y. Chujo, *Mater. Chem. Front.* **2018**, *2*, 573–579. 3) J. Ochi, K. Tanaka, Y. Chujo, *Angew. Chem. Int. Ed.* **2020**, *59*, 9841–9855.