Crystalline Framework Composed of Benzo[e]pyrenedicarboxylic Acid

(¹*Graduate School of Engineering, Osaka University*, ²*ICS-OTRI, Osaka University*) OSvetlana Em,¹ Katsuaki Iwasa,¹ Maiki Nishimoto,¹ Yumi Yakiyama,^{1,2} Hidehiro Sakurai^{1,2} **Keywords**: Pyrene; Porous Molecular Crystal; Hydrogen Bond

Porous materials organic composed via weak intermolecular interactions such as hydrogen bonds¹⁾ are receiving significant interest due to their softer structure compared to metal- or covalent-organic frameworks (MOFs and COFs). This makes them more flexible and responsive to stimuli. This work examined a new pyrene derivative 1 that contains a benzene dicarboxylic acid component. This derivative is used as the main building block for creating porous organic materials based on pyrene. As pyrene is known for its unique

properties such as high charge carrier mobility, light absorption, solution processability, and thermal stability²⁾, the resulting frameworks are expected to exhibit various electric properties by altering the guest molecules inside them.

Synthesis of 1 was performed with the following Scheme 1. Solution-state analysis of 1 revealed a solvatofluorochromism, indicating the presence of intramolecular donor-acceptor interactions. Single crystal X-ray analysis revealed that 1 gave two different crystal structures depending on the crystallization conditions: porous and non-porous ones (Figure 1). The tightly









Porous Structure

Figure 1. Non-porous and porous structures of 1.

packed non-porous structure was stabilized by hydrogen bond, π - π , and CH- π interactions, while the porous one mainly relied on the former two.

1) Hisaki, I.; Xin, C.; Takahashi, K.; Nakamura, T. *Angew. Chem. Int. Ed.* **2019**, *58*, 11160. 2) Kinik, F. P.; Ortega-Guerrero, A.; Ongari, D.; Ireland, C. P.; Smit, B. *Chem. Soc. Rev.* **2021**, *5*, 3143.