



## Molecular Porous Host•Guest Crystals

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Recently, porous organic crystals (**POC**) based on macrocycles have shown exceptional sorption and separation properties.<sup>1</sup> Yet, the impact of guest presence inside a macrocycle prior to crystallization and adsorption has not been studied. We will show that the inclusion of trimethoxybenzyl-azaphosphatane in the macrocycle cucurbit[8]uril (CB[8]) affords molecular porous host•guest crystals (**PHGC**) with radically new properties.<sup>2</sup> Not only the guest could tune the porous space of CB[8] crystals, but also unactivated hydrated **PHGC** could adsorb iodine spontaneously and selectively at room temperature and atmospheric pressure. The absence of (i) heat for material synthesis, (ii) moisture sensitivity, and (iii) energy-intensive steps for pore activation are attractive attributes to produce porous materials at low energetic costs. <sup>1</sup>H NMR and DOSY were instrumental for monitoring the H<sub>2</sub>O/I<sub>2</sub> exchange and iodine-doped crystals showed markedly different second harmonic generation (SHG).

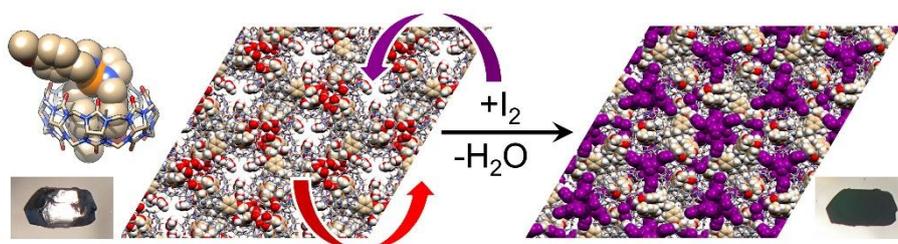


Figure 1. Host•guest complex with CB[8], packing showing 1D channels and iodine adsorption.

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<sup>1</sup> H. Zhu, L. Chen, B. Sun, M. Wang, H. Li, J. F. Stoddart, F. Huang, *Nat. Rev. Chem.* **2023**, 7, 768-782.

<sup>2</sup> X. Yang, C. Li, M. Giorgi, D. Siri, X. Bugaut, B. Chatelet, D. Gigmes, M. Yemloul, V. Hornebecq, A. Kermagoret, S. Brasselet, A. Martinez, D. Bardelang, *Angew. Chem. Int. Ed.* **2022**, 61, e202214039.