

# Diamino-4,4-bithiazoleが形成するホスト-ゲスト結晶とゲスト吸着に伴うダイナミックな分子運動

(東北大多元研) 西山浩、星野哲久、武田貴志、芥川智行、(北大電子研) 高橋仁徳、野呂真一郎、中村貴義

## Host-Guest Molecular Crystals of Diamino-4,4-bithiazole and Dynamic Molecular Motions via Guest Sorption

Hiroshi Nishiyama, Norihisa Hoshino, Takashi Takeda, Kiyonori Takahashi, Shin-ichiro Noro, Takayoshi Nakamura, and Tomoyuki Akutagawa

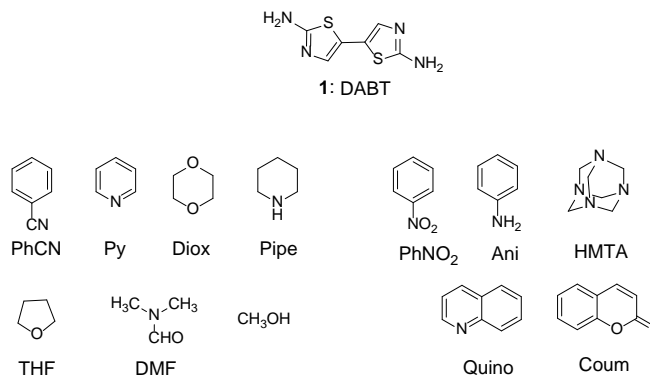


Figure 1. Molecular structure of host 1 and Various guest molecules.

ジアミノ-4,4-ビチアゾール (1) は、ピリジン、ベンズニトリルなどの様々な有機化合物とホスト-ゲスト錯体を形成する。可逆なゲスト吸着-脱着過程は、室温における粉末結晶への気相拡散と加熱による脱着で実現される。水素結合性の分子集合体 1 は、柔軟な結晶格子を有し、分子配列様式のダイナミックな変化が、ゲスト分子の極性に応じて生じた結果である。

Diamino-4,4-bithiazole (1) formed host-guest binary molecular crystals with various types of organic guest molecules including pyridine (Py), benzonitrile (PhCN), etc. Reversible molecular adsorption-desorption responses were observed with guest molecules around room temperature as the crystalline powder were heated during the desorption process and exposed to guest vapor during the re-adsorption process. The hydrogen-bonding molecular assemblies of 1 demonstrated lattice flexibly via the configuration change in the molecular arrangements according to the size and polarity of the guest molecules.

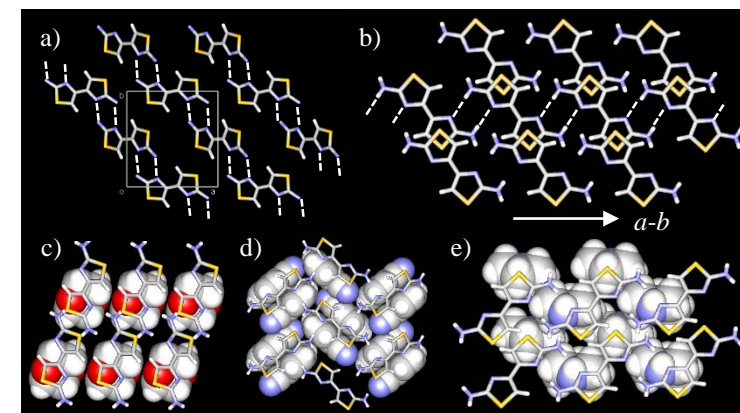


Figure 2. Variation of the hydrogen-bonded packing structures of 1. a) Isolated 1D-chain in crystal 1•(THF)<sub>2</sub>. b) 2D sheet in 1•(CH<sub>3</sub>OH)<sub>2</sub>. c) 2D sheet in crystal 1•(Diox). d) 2D herringbone in crystal 1•(PhCN)<sub>2</sub>. e) Isolated double 1D chains in 1•(Pipe)<sub>2</sub>.