

ピリジン置換 TTF の PF_6^- 塩が形成する水素結合ダイマーの固体構造と電子状態

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Solid-state Structure and Electronic States of Hydrogen-bonded Dimer of Pyridyl-substituted Tetrathiafulvalene Salted with PF_6^-

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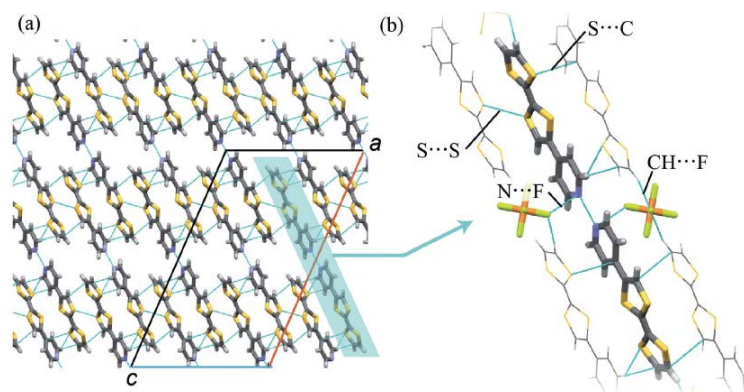


Figure 1. 結晶内におけるパッキング様式(a)と分子間相互作用(b)

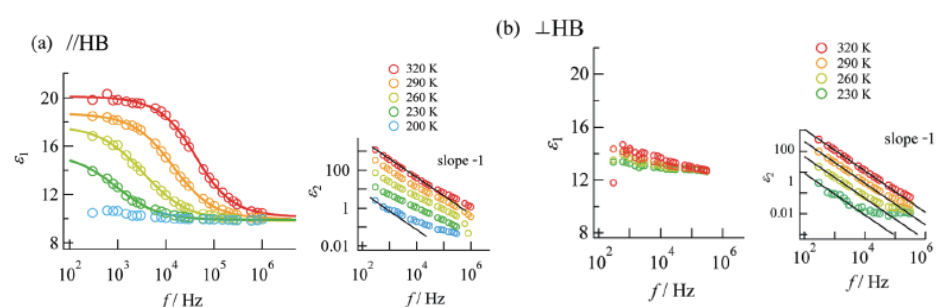


Figure 2. 単結晶試料を用いた水素結合に平行(a)および垂直(b)方向の誘電率の温度一周波数依存性

分子間水素結合サイトを有するTTFPyの PF_6^- 塩は水素結合性ダイマーを形成し、ピリジンユニット間のプロトン揺らぎに起因した誘電率の異方性を占めず。この誘電異常は、デバイ型の誘電緩和で説明可能であり、TTFPy分子の電子分極とのカップリングにより水素結合ネットワークの誘電応答を二倍程度増幅する。

Hydrogen bonding was investigated in a newly prepared salt of pyridyl-substituted tetrathiafulvalene (TTFPy) that formed a dimer structure by hydrogen bonding and was salted with PF_6^- anions. An anisotropic dielectric anomaly was observed owing to local proton transfer between two pyridyl moieties. This behavior was well explained by a model of Debye-type dipole relaxation, the dipole moment in a network of TTFPy/ H^+ /TTFPy dimers was amplified by a factor of 2 owing to coupling with the electronic polarization of TTFPy moieties.