

Synthesis and characterization of two organic cation hydrogensulfates: 1-(2,5-dimethylphenyl)piperazine-1,4-dium bis(hydrogensulfate) monohydrate (SI) and 1-(2,3-dimethylphenyl) piperazine-1,4-dium bis(hydrogensulfate) (SII).

Autorzy

M. Arbi

Lamia Khedhiri

Maciej Wojtaś

Erwann Jeanneau

Frederic Lefebvre

Chérif Ben Nasr

Rok wydania

2017

CzasopismoJournal of Molecular
StructureNumer woluminu

1134

Strony

625-637

DOI

10.1016/j.molstruc.2016.12.099

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Treatment of 1-(2,5-dimethylphenyl)piperazine and 1-(2,3-dimethylphenyl)piperazine with H₂SO₄ in 2:1 molar ratio at RT affords the corresponding sulfate salts [C₁₂H₂₀N₂][HSO₄]₂·H₂O (SI) and [C₁₂H₂₀N₂][HSO₄]₂ (SII). These compounds have been characterized by X-ray diffraction, thermal analysis and spectroscopic investigations (IR and NMR). In the atomic arrangement of (SI) the HSO₄⁻ anions are associated by pairs linked to the water molecules forming corrugated ribbons, while in the (SII) structure, the pairs of the HSO₄⁻ anions form corrugated chains. Solid-state ¹³C and ¹⁵N CP-MAS NMR spectroscopies are in agreement with the X-ray structure. The vibrational absorption bands were identified by infrared spectroscopy. NMR peaks were attributed with the aid of DFT calculations. The electronic properties such as HOMO and LUMO energies were determined.

Słowa kluczowe

x-ray diffraction, crystal structure, CP-MAS NMR, infrared spectroscopy, Thermal analysis

Adres publiczny

<http://dx.doi.org/10.1016/j.molstruc.2016.12.099>

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-08-24 08:49:07

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/726AYHh>.