



Structures and phase transitions in molecular complexes containing tetrafluoroboric acid and tetramethylpyrazine.

Autorzy

Magdalena Rok

Przemysław Szklarz

Grażyna Bator

Rok wydania

2018

Czasopismo

CrystEngComm

Numer woluminu

20

Strony

5772-5781

DOI

10.1039/c8ce01231h

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Crystals of tetrafluoroboric acid with tetramethylpyrazine, TMP + HBF₄ + H₂O (1 : 1 : 2, **A**), TMP + HBF₄ (1 : 1, **B**) and TMP + HBF₄ (1 : 2, **C**) were synthesized and characterized by physicochemical experimental methods. The crystal structures for **A** and **B** were determined at 100 K. Since **C** undergoes a phase transition at 217/223 K (cooling/heating) the structures were measured at 100 and 250 K. Infinite chains of molecules linked via the hydrogen bonds are present in the crystals **A** and **B**. A BF₄⁻...TMPH₂²⁺...BF₄⁻ assembly was found in the crystal structure of **C**. The dielectric responses have been measured for all three crystals, **A**, **B** and **C**, in a wide temperature (160–300 K) and frequency range (100 Hz–2 MHz). The mechanism of the phase transition at 217/223 K found in **C** as well as the origin of the ac conductivity was determined to be related to the dynamics of protons in the hydrogen bonds.

Adres publiczny

<http://dx.doi.org/10.1039/c8ce01231h>

Strona internetowa wydawcy

<https://www.rsc.org/>