Struktur Garam 1,3-Dimethyl-1,2,3-benzotriazolium Hexafluoroposfat (Kajian Interaksi Sekunder Kation-Anion dalam Cairan Ionik)

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Abstract

Chemical preparation, characterization, thermal analysis and X-ray single crystal investigation of 1,3-dimethyl-1,2,3-benzotriazolium hexafluorophosphate "ionic liquid" salt are described. The compound crystallizes in the monoclinic system with Cc space group. Its unit cell dimensions are a = 1221.46(9) pm, α = 90°, b = 1073.22(8) pm, β = 102.098(2)°, c = 869.73(6) pm, γ = 90°, V = 1.11480(14) nm^3 and Z = 4. The crystal structure can be described as a typical layered organization built by all the components of the structure. Connection in these layers are established by CH···F and CH···N hydrogen bonds.

Key Words: ionic liquids, thermal analysis, X-ray single crystal and 1,3-dimethyl-1,2,3-benzotriazolium hexafluorophosphate.

Abstrak

Telah dilakukan preparasi, karakterisasi, analisa termal dan penentuan struktur kristal tunggal "cairan ionik" garam 1,3-dimethyl-1,2,3-benzotriazolium hexafluoroposfat. Senyawa ini mengkristal dalam sistem monoklin dengan kelompok ruang Cc. Unit dimensi kristalnya adalah a = 1221.46(9) pm, α = 90°, b = 1073.22(8) pm, β = 102.098(2)°, c = 869.73(6) pm, γ = 90°, V = 1.11480(14) nm^3 and Z = 4. Struktur kristal dapat digambarkan sebagai struktur berlapis antara rantai kation dan rantai anion. Antar lapisan dihubungkan oleh adanya ikatan hidrogen CH···F dan CH···N.

Kata Kunci: cairan ionik, analisa termal, struktur kristal tunggal dan 1,3-dimethyl-1,2,3-benzotriazolium hexafluoroposfat.