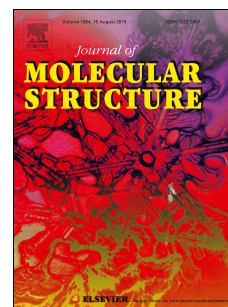


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Structural, vibrational and electrical studies of tetramethylammonium trichloromercurate $[(\text{CH}_3)_4\text{N}]\text{HgCl}_3$

F. Lambarki⁽¹⁾, A. Ouasri^(1,2*), A. Rhandour⁽¹⁾, M. Saadi⁽³⁾, L. El Ammari⁽³⁾ and L. Hajji⁽⁴⁾

⁽¹⁾ Laboratoire de physico-chimie des matériaux inorganiques, Université Ibn Tofail, Faculté des Sciences, B. P. 133, 14000 Kenitra, MAROC

⁽²⁾ Centre Régional des Métiers de l'Education et de la Formation, Madinat Al Irfane, Souissi, BP 6210 Rabat, Morocco.

⁽³⁾ Laboratoire de Chimie Appliquée des Matériaux, Centre des Sciences des Matériaux, Faculty of Sciences, Mohammed V University in Rabat, Avenue Ibn Batouta, B.P. 1014, Rabat, Morocco

⁽⁴⁾ LMCN, Faculty of Sciences and Technologies, University Cadi Ayyad Marrakech, Morocco

Abstract

The crystal structure of $[(\text{CH}_3)_4\text{N}]\text{HgCl}_3$ is redetermined at 298 K in monoclinic system $[P2_1(Z = 4); a=7.5501(3) \text{ \AA}, b=15.6871(6) \text{ \AA}, c=8.8666(4) \text{ \AA}, \beta=93.575(2)^\circ]$. The anionic sublattice of the crystal is consisted of $(\text{HgCl}_3^-)_n$ polyhedra sharing a vertex to form zigzag chains along the a-axis. The crystal structure cohesion is ensured by C--H...Cl hydrogen bonds that connect organic $(\text{CH}_3)_4\text{N}^+$ and mineral parts. Infrared ($450\text{--}4000 \text{ cm}^{-1}$) and Raman ($50\text{--}3500 \text{ cm}^{-1}$) spectra, studied at room temperature, confirm the connection of organic cations $(\text{CH}_3)_4\text{N}^+$ and $(\text{HgCl}_3^-)_n$ polymers by C-H...Cl hydrogen bonding. One phase transition is observed and studied for this compound by DSC ($269^\circ/260^\circ\text{C}$) and dielectric measurements (254°C). The dielectric constant evolution with temperature indicates that the observed transition is of ferro-paraelectric type. Cole-Cole plots of impedance complex have been performed. The activation energy (0.85 eV) obtained from dc conductivity analysis indicates a probable hopping mechanism of the transport in the title compound.

Keywords: Tetramethylammonium, trichloromercurate, crystal structure, X-Ray diffraction, IR, Raman, impedance complexe spectroscopy, dielectric constant, Cole-Cole plots.

* Corresponding author: aouasri@yahoo.fr (A. Ouasri)

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