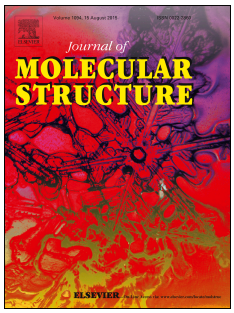
Accepted Manuscript



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PII: S0022-2860(18)30870-6

DOI: 10.1016/j.molstruc.2018.07.051

Reference: MOLSTR 25456

To appear in: *Journal of Molecular Structure*

Received Date: 13 May 2018

Revised Date: 10 July 2018

Accepted Date: 16 July 2018

Please cite this article as: F. Lambarki, A. Ouasri, A. Rhandour, M. Saadi, L. El Ammari, L. Hajji, Structural, vibrational and electrical studies of tetramethylammonium trichloromercurate $[(CH_3)_4N]HgCl_3$, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.07.051.

Structural, vibrational and electrical studies of tetramethylammonium trichloromercurate $[(CH_3)_4N]HgCl_3$

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Abstract

The crystal structure of $[(CH_3)_4N]HgCl_3$ is redetermined at 298 K in monoclinic system [$P2_1$(Z = 4); a=7.5501(3) Å, b=15.6871(6) Å, c=8.8666(4) Å, β=93.575(2)°]. The anionic sublattice of the crystal is consisted of $(HgCl_3^-)_n$ 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 $(CH_3)_4N^+$ and mineral parts. Infrared (450–4000 cm^{-1}) and Raman (50–3500 cm^{-1}) spectra, studied at room temperature, confirm the connection of organic cations $(CH_3)_4N^+$ and $(HgCl_3^-)_n$ polymers by C-H…Cl hydrogen bonding. One phase transition is observed and studied for this compound by DSC (269°/260°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 hoping 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**.**

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