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Short communication

Crystal structure, physical study and Hirshfeld surface analysis of $(C_9H_{26}N_4)[SnCl_6]Cl_2{\cdot}2H_2O$

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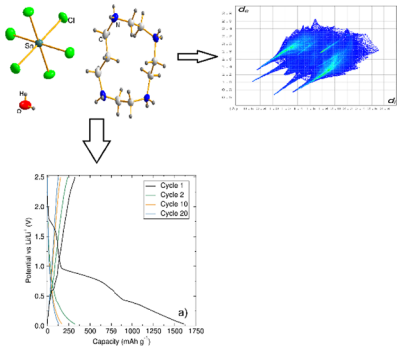
GRAPHICAL ABSTRACT

Hirshfeld surface illustrating the presence of the shortest reciprocal C—HC… HC—C/C—HC… HC—C interactions. Galvanostatic cycling of the $(C_9H_{28}N_4)[SnCl_6]Cl_2{\cdot}2H_2O$ at a constant current of 100 mA g^{-1} with potential limitation between 0.30 and 2.5 V.



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ABSTRACT

$(C_9H_{26}N_4)[SnCl_6]Cl_2{\cdot}2H_2O$ has been synthesized in solution and its structure confirmed by single-crystal X-ray diffraction. It crystallizes in the monoclinic system, with space group $P2_1/n$ (14), Z = 4, with refined cell parameters (Å,°) a = 10.7550(3), b = 15.3981(7), c = 13.8750(5), β = 103.095(3), V = 2238.04(15) $Å^3$. The 3D framework of the title compound is made of free molecules 1,4,7,10-tetraazacyclotridecane, $[SnCl_6]$, Cl atoms and water molecules, interacting through an intricate network of hydrogen-bonds and H…Cl interactions. The 1,4,7,10-tetraazacyclotridecane moiety is also confirmed by Raman spectroscopy. The Hirshfeld surface analysis of $(C_9H_{26}N_4)[SnCl_6]Cl_2{\cdot}2H_2O$ is elucidated. Preliminary investigations of the electrochemical performance of the title compound as an active material in a Li-ion battery have also been carried out.

1. Introduction

Macrocycles are synthetic or natural polydentate ligands, with their donor atoms incorporated in a cyclic backbone or/and in substituents attached to it. They contain a cyclic framework of at least twelve atoms. Naturally occurring macrocycles can however reach even more than 50

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