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Crystal structure, Hirshfeld surface analysis, thermal behavior and spectroscopic investigations of a new organic cyclohexaphosphate, $(C_{10}H_{15}N2)4(Li)2(P6\ O_{18})(H_2O)6$.

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Streszczenie

The synthesis and the structure of (C10H15N2)4(Li)2(P6O18)(H2O)6 are described. This compound crystallizes in the triclinic system, with the centric space group P-1 and the following unit cell parameters: a=9.7762(6), b=10.2502(8), c=15.2173(11) Å, α=92.588(4), β=98.855(4), γ=115.724(4)°, Z=2 and V=1346.62(17) Å3. The crystal structure has been solved and refined to R=0.0452 and Rw=0.1121. [Li2(P6O18)(H2O)]4- entities are associated by strong OH···O hydrogen bonds to form inorganic layers lying in the (a, b) plane. These layers are interconnected with the organic entities via NH···O and CH···O hydrogen bonds. In this atomic arrangement, H bonds between the different species play an important role in the three-dimensional network. The contacts enrichment ratios derived from the Hirshfeld surface analysis show that the crystal packing is stabilized by ionic bridges Li+ … O, strong N/OH···O hydrogen bonds but also hydrophobic interactions between the two independant 1-phenylpiperazine-1,4-dium ligands. The Molecular Electrostatic Potential (MEP) maps and the HOMO and LUMO energy gaps of the new compound were computed. The title compound was further characterized by FT-IR and NMR spectroscopies. The crystal symmetry was confirmed by 31P and 7Li MAS NMR and the vibrational absorption bands were identified by infrared spectroscopy. The new compound was also characterized by thermal analysis to determine the thermal behavior.

Słowa kluczowe

Cyclohexaphosphate, X-ray diffraction analysis, Hirshfeld surfaces, Enrichment ratio, MAS-NMR spectroscopy, Thermal analysis

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