

Crystal structure, Hirshfeld surface analysis, thermal behavior and spectroscopic investigations of a new organic cyclohexaphosphate, $(C_{10}H_{15}N_2)_4(Li)_2(P_6O_{18})(H_2O)_6$.

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The synthesis and the structure of $(C_{10}H_{15}N_2)_4(Li)_2(P_6O_{18})(H_2O)_6$ 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, $\alpha=92.588(4)$, $\beta=98.855(4)$, $\gamma=115.724(4)^\circ$, $Z=2$ and $V=1346.62(17)$ Å³. The crystal structure has been solved and refined to $R=0.0452$ and $R_w=0.1121$. $[Li_2(P_6O_{18})(H_2O)]_4^-$ entities are associated by strong $OH\cdots O$ hydrogen bonds to form inorganic layers lying in the (a, b) plane. These layers are interconnected with the organic entities via $NH\cdots O$ and $CH\cdots O$ 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 $Li^+ \cdots O$, strong $N/OH\cdots O$ hydrogen bonds but also hydrophobic interactions between the two independent 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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