HYDROTHERMAL SYNTHESIS AND CRYSTAL STRUCTURE OF $[Zn(pytpy)_2][NO_3]_2 \cdot 2H_2O$

Yu Ding,[1] Feng Wang,[2] Zong-Jun Ku,[1] Lian-Sheng Wang,[1] and Huan-Bo Zhou[1]

UDC 548.736

The title compound, $[Zn(pytpy)_2][NO_3]_2 \cdot 2H_2O$ (pytpy = 4′-(4-pyridyl)-2,2′: 6′,2″-terpyridine), has been synthesized by the reaction of $Zn(NO_3)_2 \cdot 6H_2O$ with pytpy, and its crystal structure was determined by single-crystal X-ray diffraction. The crystal belongs to tetragonal space group $P4_3$ with a = 0.90873(8) nm, b = 0.90873(8) nm, c = 4.4741(6) nm, V = 3.6946(7) nm^3, Z = 4, D_c = 1.521 g/cm^{-3}, μ = 0.736 mm^{-1}, $F(000)$ = 1744, R = 0.0871, wR = 0.1302 for 5553 observed reflections with $I > 2\sigma(I)$. X-ray analysis has revealed that the Zn^{II} ion is surrounded by six N atoms from two pytpy ligands leading to a distorted octahedral geometry. In the crystal structure there are numerous strong intermolecular and intramolecular H-bonds and π–π interactions.

Keywords: pytpy, zinc complex, crystal structure, hydrothermal synthesis.