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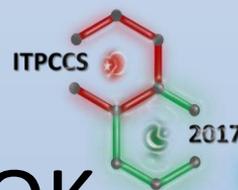
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ABSTRACT E-BOOK



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The role of intermolecular interactions in the assembly of the lead coordination polymer containing carboxylate ligand

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A new Pb(II) complex with m-toluic acid ligand has been synthesized and structurally characterized by FT-IR, ¹H NMR, ¹³C NMR spectroscopic techniques and single crystal X-ray diffraction studies. Crystal data for the title complex: C₁₆H₁₆O₅Pb, monoclinic, space group P21/c (no. 14), a = 10.872(4) Å, b = 7.181(2) Å, c = 20.739(9) Å, β = 100.595(19)°, V = 1591.4(10) Å³, Z = 4, T = 100 K, μ(Mo Kα) = 10.624 mm⁻¹, Dcalc = 2.0679 g/cm³, 51344 reflections measured (6° ≤ 2θ ≤ 61.86°), 4826 unique (Rint = 0.2474, Rsigma = 0.0806) which were used in all calculations. The final R1 was 0.1016 (I ≥ 2σ(I)) and wR2 was 0.1552 (all data). (Figure 1a). The study of X-ray single crystal diffraction revealed that the title complex display a polymeric structure and in polymeric structure the carboxylate groups exhibit two different coordination modes with Pb²⁺ ions: η² chelating and μ²-η²:η¹ chelating bridging modes, forming one dimensional polymeric chain [1]. Our analyses also revealed that the substantial role of intermolecular hydrogen bonds, C-H...π and π...π stacking interactions in the assembly of the polymeric chains in title complex. In addition, these intermolecular contacts in the title complex have been examined based on the Hirshfeld surfaces and their associated 2D fingerprint plots (Figure 1b).

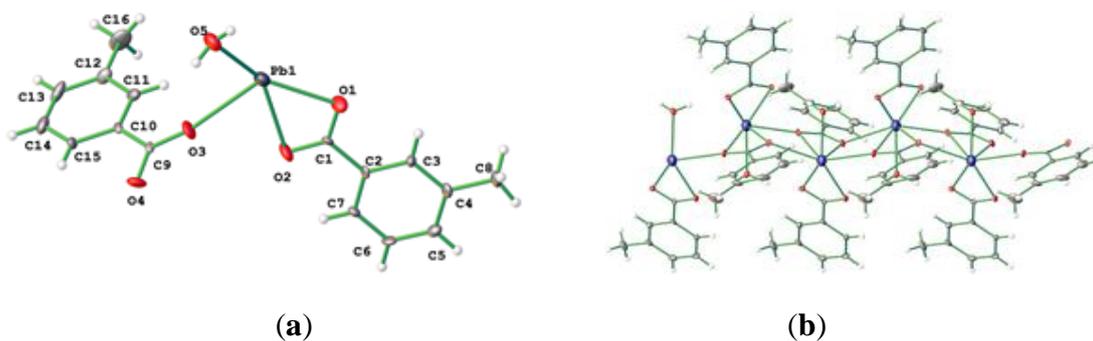


Figure 1: (a) Asymmetric molecular unit of title complex with the selected numbering scheme, (b) 1D polymeric unit of title complex

References

[1] D. Hazari *et al.*, *Inorg chem commun* **65**: 1-3(2016)