

and totally protonated acid $\text{Cs}(\text{H}_2\text{C}_2\text{O}_4)(\text{HC}_2\text{O}_4)(\text{H}_2\text{O})_2$ [4]. We focus here on the structural reinvestigation of a caesium oxalate at 100 K. The structure is resolved in the space group $P2_1/c$, with the lattice parameters consistent with the data reported in [3], ($a=10.3677(10)\text{\AA}$, $b=6.7050(15)\text{\AA}$, $c=6.5849(8)\text{\AA}$, $\alpha=93.552(4)^\circ$). However, the new XRD structural study shows that instead of the chemical formula suggested in [3], the compound contains both the acid and the dianion: $\text{Cs}_2(\text{H}_2\text{C}_2\text{O}_4)(\text{C}_2\text{O}_4)$.

The asymmetric unit contains one Cs atom, one half oxalate dianion (C(1)O(1)O(2)) and one half oxalic acid molecule [C(2)O(3)O(4)H]. The nine-coordinated caesium atom is surrounded by four centrosymmetrical $\text{H}_2\text{C}_2\text{O}_4$ molecules, acting in unidentate fashion, and four oxalato ligands. The dianion is involved in a chelation by one function and in unidentate mode by the second function. The 2D structure consists of double files of CsO_6 polyhedra, running along [001] and [010] directions. In the two kinds of files, each polyhedron is sharing one edge with its nearest neighbours forming layers of double files. Within the layers, the deprotonated ligands link the files, while the other ligands connect the double file layers.

The single H atom has been localized in the difference Fourier map. In this structure, it is noteworthy to point out that, in each kind of ligand, it occurs a distance C-OH longer than the others C-O distances, implying a vicinity of the proton near the O1 or O4 atom. Strong H-bonds involving O4 and/or O1, occur between acid molecules and oxalate anions, leading to files extending along [100] direction. Further studies should concern the H motion, eventually by H RMN and electrical conductivity.

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Carbon nanotubes as nucleation agents in polypyrrole-carbon nanotube nanocomposites

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A nanocomposite has been synthesized by *in-situ* chemical polymerization using pyrrole (Py) as a monomer and single wall carbon nanotube (SWNT) as an additive component. Experiments show that PPy growth on the surface of SWNTs in the spherical and cylindrical core-shell structures. As a result of strong bonds with carbon nanotubes (CNTs) [1, 2], the radical monomers and oligomers forming during the polymerization are adsorbed and anchored on amorphous carbon and SWNT surfaces which act as preferable sites for nucleation and growth of PPy. Depending on the anchoring sites the growth modes give rise to different morphologies. Wide-angle X-ray diffraction patterns indicate a change in the crystallinity of PPy in the composite.

The FTIR and Raman spectra of PPy/SWNTs composites consist of a broad adsorption band in the special domain between 4000 and 2500 cm^{-1} , which is commonly assigned for the adsorption band of O-H, C-H, N-H groups. However, due to the intensity of this adsorption band relatively increases with the laser excitation intensity, a portion of the 3000-3500 cm^{-1} band is speculated as the photoluminescence arising from transitions between valence band to polaron or to bipolaron levels [3]. Charge transfer interaction between composite components likely brings

more new polaron and bipolaron levels into the band gap of PPy.

The Raman spectra of the composite show the change in 1590, 1280 cm^{-1} and 940 cm^{-1} peaks. The band located at about 940 cm^{-1} is assigned to the ring deformation associated with radical cation (polaron state) while the band around 1590 cm^{-1} is the tangential mode (G-band) associated with sp^2 -hybridized carbon atoms (C=C bond) of SWNTs and PPy. The 1280 cm^{-1} band in PPy/SWNTs is assumed to be the superposition of both 1310 and 1253 cm^{-1} bands which stand for the bipolaron state of PPy [4, 5]. The decline of 940 cm^{-1} band and the emergence of 1280 cm^{-1} band in Raman spectra then indicate the transition from polaron to bipolaron state, i.e., indicate an increase in conductivity of PPy.

The UV-Vis spectra of PPy and PPy/SWNTs show two major peaks centering around 340 nm and 460 nm. The 340 nm adsorption band stands for $\pi^*-\pi$ transition while the 460 nm adsorption band represents the bipolaronic transition in PPy relating to the oxidized levels. The 340 nm band is intensified and undergoes a redshift while the 460 nm band exhibits a blueshift when SWNTs are doped. The change in the intensity and position of these adsorption bands indicates a strong modification in electronic structure and polaron levels in PPy bandgap.

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Molecular structure of binuclear Ag (I) complex of phenyl bis(2-pyridyl)phosphine

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The design of silver (I) complexes has attracted particular attention due to their interesting structures, photoluminescent, biological and pharmacological activities, such as anticancer and antifungal properties [1] we describe synthesis, spectroscopic studies and crystal structure of Ag(I) complex of phenyl bis(2-pyridyl)phosphine. This complex was synthesized by reacting 2-lithiopyridine and dichlorophenyl phosphine in Et_2O [2] ($\text{PhP}(2\text{-py})_2$) followed by treating with AgNO_3 in water. Single-crystal X-ray analysis reveals that mentioned complex crystallizes in monoclinic system, with $P2_1/n$ space group. The structure of this complex consists of two silver atoms, two molecules of ligand that act as tridentate beside two nitrate ions. The $\text{Ag}\cdots\text{Ag}$ distances is 3.216 (9) \AA , which is shorter than the sum of the van der Waals radii of two silver atoms (3.44 \AA), suggesting the existence of metal-metal interaction between the silver atoms. The free oxygen atoms of nitrate ligands interact with hydrogen atoms of the pyridyl groups to form hydrogen bonding. The separations for C(2) \cdots O(3), C(3) \cdots O(2), C(8) \cdots O(1) and C(10) \cdots O(3) (symmetry code: 1/2+x, 3/2-y, 1/2+z, 5/2-x, -1/2+y, 3/2-z and -1+x,y,z) are 3.369(8), 3.355(8), 3.313(8) 3.332(8) \AA .

In order to verify presence of silver-silver intra-molecular bonding the electron density of the synthesized complex was studied in the context of Quantum Theory of Atoms in Molecules, QTAIM[3]. The electron density of the complex was obtained from a single point energy calculation on the X-ray resolved crystal structure by Win-GAMESS.08 suite of programs at the B3LYP combined with three different basis sets for different elements; 6-31G for carbon and hydrogen atoms, 6-31+G(d) for nitrogen, oxygen and phosphorus and DZVP (DFT orbitals)