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Title:	Schiff base driven denticity-fluctuated structural assortment of zinc-pseudohalide complexes: synthesis, structures and electrical transport properties
Authors:	Singla, Labhini (/jspui/browse?type=author&value=Singla%2C+Labhini) Choudhury, Angshuman Roy (/jspui/browse?type=author&value=Choudhury%2C+Angshuman+Roy)
Keywords:	Schiff base pseudohalide electrical transport
Issue Date:	2022
Publisher:	Royal Society of Chemistry
Citation:	CrystEngComm, 24(13), 2418-2428
Abstract:	<p>We report the peculiar characteristics of a polydentate Schiff base towards zinc(II) ions in the presence of pseudohalides (thiocyanate and azide) and the charge transport properties of zinc complex mediated devices in the solid state. The designed polydentate chelator, [HL = (Z)-2-methoxy-6-(((2-methoxy phenyl)imino)methyl)phenol]], was synthesized by coupling of o-anisidine and o-vanillin in ethanol under reflux, and the ligand was isolated in a single-crystalline phase in an orthorhombic system with the Pbc<sub>a</sub> space group. Interestingly, the ligand bears unique structural features towards the coordination with zinc ions in the presence of thiocyanate and azide ions leading to mononuclear and dinuclear zinc-Schiff base-pseudohalide complexes (ZnP11NCS and ZnP11N3), respectively. In the ZnP11NCS complex, the Schiff base ligand becomes protonated to a zwitterionic form, which causes their monodentate/bidentate behaviour towards Zn(II) ions. In contrast, the ligand, P11, under identical reaction conditions, behaves as a tridentate chelating ligand towards Zn(II) ions in the ZnP11N3 complex having a symmetric <math>\mu_1,1</math>-phenoxo-bridge. In both complexes, NCS and N3 ions coordinate with Zn(II) ions in a terminal coordination mode. Crystal engineering approaches and Hirshfeld surface and energy framework analysis of the complexes delineate the dominant contribution of H...S and H...N hydrogen bonding and C-H...<math>\pi</math> interactions for a structural assortment of the compounds. Further, the complexes have been employed to construct devices to explore the charge transport properties in the dark and a shower of photons. The ZnP11N3 complex exhibits better charge transport properties than ZnP11NCS as evident from high DC conductivity measurement values and relaxation times caused by optical phonon activation under dark and light conditions. This feature might be utilized to explore their template applications in designing electronic devices as per the industry's needs.</p>
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