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Title:	Novel primary amide-based cationic metal complexes: green synthesis, crystal structures, Hirshfeld surface analysis and solvent-free cyanosilylation reaction
Authors:	Markad, D. (/jspui/browse?type=author&value=Markad%2C+D.) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Cationic Metal Hirshfeld Surface Analysis Crystal Structures
Issue Date:	2019
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Citation:	Dalton Transactions,48(11), pp. 3743-3757.
Abstract:	<p>A new symmetrical and flexible primary amide functionalized ligand, 2,2'-(ethane-1,2-diylbis((pyridin-2-ylmethyl)azanediyl))diacetamide (2-BPEG), has been synthesized and structurally characterized. Using this multidentate ligand, four novel metal complexes, namely [Cu(2-BPEG)](ClO₄)₂·0.5H₂O (1), [Zn(2-BPEG)](ClO₄)₂ (2), [Zn(2-BPEG)](ZnCl₄)·H₂O (3) and [Cd(2-BPEG)(H₂O)](ClO₄)₂·H₂O (4), have been synthesized under ambient conditions and characterized by elemental, spectroscopic and thermal analysis, and single and powder X-ray diffraction. Complexes 1–3 are hexacoordinated with an N₄O₂ donor set (provided by the hexadentate 2-BPEG ligand), while complex 4 is heptacoordinated with an additional coordinated water molecule. In all cases, the 2-BPEG ligand acts as a hexadentate ligand. A change in the starting metal salt has resulted in the formation of 2 and 3 with different tetrahedral anions, ClO₄[–] and ZnCl₄[–], respectively. This has provided an opportunity to showcase anion-directed supramolecular networks for these compounds. Compounds 1, 2 and 4 with perchlorate anions show similar and comparable intermolecular interactions in their 3D networks. On the other hand, the supramolecular self-assembly of 3 is dominated by a variety of intermolecular interactions such as C–H...Cl, N–H...Cl, O–H...Cl and C–H...O due to the presence of a tetrachlorozincate(II) ion. Moreover, the role of weak intermolecular interactions in the crystal packing has been analysed and quantified using Hirshfeld surface analysis. Furthermore, compound 4 exhibiting an open Lewis acid site has been found to be a very efficient and recyclable heterogeneous catalyst for the solvent-free cyanosilylation of various aldehydes with trimethylsilyl cyanide (TMSCN) producing the corresponding trimethylsilyl ether in high yields.</p>
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