IMIDAZOLE-FUNCTIONALIZED PYRIDINIUM-FUSED SELENADIAZOLIUM SALTS AS VERSATILE CHALCOGEN BOND DONORS

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Abstract. Novel imidazole-functionalized pyridinium-fused selenadiazolium salts were synthesized and structurally characterized as versatile chalcogen bond (ChB) donors. The compounds were obtained from the reaction of 2-pyridylselenyl chloride with 4,5-dicyanoimidazole, yielding a monocationic chloride salt and a dicationic perrhenate derivative. X-ray diffraction analysis revealed that both salts adopt nearly planar selenadiazole cores and T-shaped geometries stabilized by intramolecular Se···X (X = Cl, O) chalcogen bonds. In the solid state, monocationic salt forms a supramolecular polymer *via* a combination of $[Se\cdots Cl]_2$ dimerization and, secondary, Se···N chalcogen bonds involving the imidazole moiety. Theoretical QTAIM and RDG analyses confirmed the presence and attractive nature of key noncovalent interactions (Se···Cl, Se···N, Se···O, H···Cl, H···O), with estimated energies consistent with typical chalcogen and hydrogen bonds. This work illustrates a rational strategy for managing supramolecular organization through synergistic noncovalent interactions, offering a pathway toward predictable chalcogen-bond-driven architectures for crystal engineering and functional materials.

Keywords: imidazole, selenadiazolium salt, supramolecular polymer, chalcogen bond, noncovalent interactions.