CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2026, 21(1), 125-135
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.ichem.md
https://doi.org/10.19261/cjm.2026.1478

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

Evgeny Dukhnovsky [a], Namiq Shikhaliyev [b*], Alexander Sapronov [a], Alexey Kubasov [c], Alexander Novikov [d], Alexander Tskhovrebov [a], Gulnaz Mirzayeva [e]

[a]*Peoples' Friendship University of Russia, 6 Miklukho-Maklaya str., Moscow, Russian Federation*
[b]*Department of Chemical Engineering, Baku Engineering University,120 Hasan Aliyev str., Baku, AZ0101, Azerbaijan*
[c]*Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, 31, Leninsky prosp., Moscow, Russian Federation*
[d]*Institute of Chemistry, Saint Petersburg State University, 7/9, Universitetskaya Nab., Saint Petersburg, Russian Federation*
[e]*Department of Chemical Technology, Recycling and Ecology, Azerbaijan Technical University, 25, H.Javid ave, Baku, Azerbaijan*
[*]*e-mail: namiqst@gmail.com, +994503225269*

Abstract. Novel imidazole-functionalized pyridinium-fused selenadiazolium salts were synthesised and structurally characterised 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 intermolecular Se···X (X = Cl, O) chalcogen bonds. In the solid state, monocationic salt forms a supramolecular polymer *via* a combination of $[Se\cdots Cl]_2$ dimerisation and, secondary, Se···N chalcogen bonds involving the imidazole moiety. Results of Hirshfeld surfaces analysis reveal that crystal packing primarily determined by intermolecular contacts involving hydrogen atoms. 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.

Received: 06 May 2026/ Revised final: 11 June 2026/ Accepted: 12 June 2026

© Chemistry Journal of Moldova
CC-BY 4.0 License