CHEMISTRY JOURNAL OF MOLDOVA
General, Industrial and Ecological Chemistry **AA-0509**

DOUBLE-LAYER SILICENE AS A MOLECULAR CONTAINER FOR ANTI-AROMATIC SYSTEMS

Oleksiy Mykhailenko [a*], Yuriy Prylutskyy [a], Ihor Komarov [a], Artur Strungar [b], Olena Mykhailenko [a], Oleksandra Lagerna [a]

[a]*Taras Shevchenko National University of Kyiv, 64, Volodymyrska str., Kyiv 01601, Ukraine*
[b]*Vernadsky National Library of Ukraine, 3, Holosiivskyi ave., Kyiv 03039, Ukraine*
[*]*e-mail: alexm-@ukr.net*

Abstract. The goal of this study was to stabilize the anti-aromatic cyclobutadiene using a double-layer silicene matrix. This research was also aimed at calculating the UV spectra for the nanosystem in different "silicene/ cyclobutadiene" ratios and deriving the association constant of the nanocomplex. The arrangement of cyclobutadiene molecules between two silicene planes was theoretically researched using the quantum-chemical methods. The principal result was the calculation of silicene UV spectra depending on the component ratios in the "host-guest" complexes. UV spectra were processed using the Benes-Hilderbrand method. The association constant of the "silicene-intercalate" system was found.

Keywords: "host-guest" nanocomplex, double silicene layer, cyclobutadiene, UV spectrum.