

The electronic absorption spectra and the structure of 6-(2-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-imidazole-4-ilazo)-1-oxo-2,5-dihydro-1*H*-benzo[4,5]imidazo[1,2-*c*] pyrimidine -7- carboxylic acid

© Olga V. Kovalchukova,^{1*+} Mikhail A. Ryabov,¹ All TahanRana Abdulila Abbas,^{1,2}
Boris E. Zaitsev,^{1*} Svetlana B. Strashinova,¹ and Oleg V. Volyansky¹

¹ Department of General Chemistry. Peoples' Friendship University of Russia. Miklukho-Maklay St., 6.
Moscow, 117198. Phone: +7 (495) 955-08-60. E-mail okovalchukova@mail.ru

² Chemistry Department. Technological Institute. Baghdad. Iraq.

*Supervising author; +Corresponding author

Keywords: electron spectroscopy, quantum-chemical calculations, PPP, PM3, benzo[4,5]imidazo[1,2-*c*]quinazoline, derivatives.

Abstract

Using spectral (electron spectroscopy) and quantum-chemical (PPP, PM3) methods we studied tautomeric and ionic forms 6-(2-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-imidazole-4-ilazo)-1-oxo-2,5-dihydro-1*H*-benzo[4,5]imidazo[1,2-*c*]pyrimidine-7-carboxylic acid. Its primary existence as non-flat CH-azo tautomer has been shown.