Synthesis, IR Spectra, and Steric Structure of Macrocycles Derived from Pyrimidine Compounds

R. R. Shagidullin, A. V. Chernova, G. M. Doroshkina, V. E. Kataev, Z. G. Bazhanova, S. A. Katsyuba, V. S. Reznik, A. S. Mikhailov, R. Kh. Giniyatullin, N. G. Pashkurov†, Yu. Ya. Efremov, and A. A. Nafikova

Arbuzov Institute of Organic and Physical Chemistry, Kazan Research Center, Russian Academy of Sciences, Kazan, Tatarstan, Russia

Received December 29, 2000

Abstract - A new macrocycle including pyrimidine fragments, 12,23,36-trimethyl-24,40-dioxo-15,33-dithia-2,9,13,22,26,35,38,39-octaazatetracyclo[32.3.1.1^{10,14}.1^{22,26}]tetraconta-1(38),10(39),11,13,23,34,36-heptaene, was synthesized. According to the data of IR and UV spectroscopy and HF/6-31G** quantum-chemical calculations, macrocyclic compounds of this series in crystal exist in the amino form, one NH group of which is likely to be involved in intramolecular hydrogen bond, and the other, in intermolacular hydrogen bond. The strength of the latter depends on the macroring size. In solution, the above structures are supplemented by conformers containing both intramolecularly H-bonded and free amino groups, predominantly with *trans* structure of the H−N−C=N fragment. The imino form of the aminopyrimidine moieties is hardly probable.