Molecular Modeling, IR Spectra and Structure of Chromenopyridinecarbonitrile Systems

I.V. Ivlieva (Peretokina), A.A. Mescherekova, L.M. Babkov, V.V. Sorokin
Saratov State University, Saratov, Russia
Corresponding author: lmbabkov@gmail,com

Chromeno[3,4-c]pyridine carbonitrile systems are the subject of intensive researches because they are biologically active. Medical applications require a good knowledge of their properties.

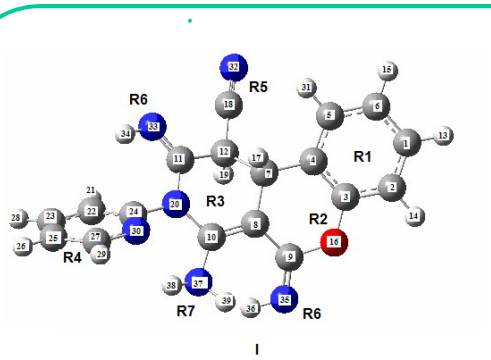
The aim of the study was to interpret the IR spectrum of a mixture of amino-imino tautomers such as 5-amino-2,4-diimino-3-(pyridine-2-yl)-2,3,4,10 b-tetrahydro-1H-chromeno[3,4-c]pyridine-1-carbonitrile (I) and 4-amino-2,5-diimino-3-(pyridine-2-yl)-2,3,5,10 b-tetrahydro-1-chromeno[3,4-c]pyridine-1-carbonitrile (II).

The main problems – modeling of the molecules, and interpretation of their IR spectrum

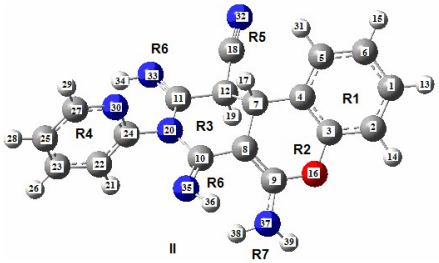
IR spectrum was measured at room temperature at Fourier Spectrophotometer Shimadzy IR at the area 400-3700 cm-1.

Method – density functional method (B3LYP/6-31 G(d))

Geometrical structure



I



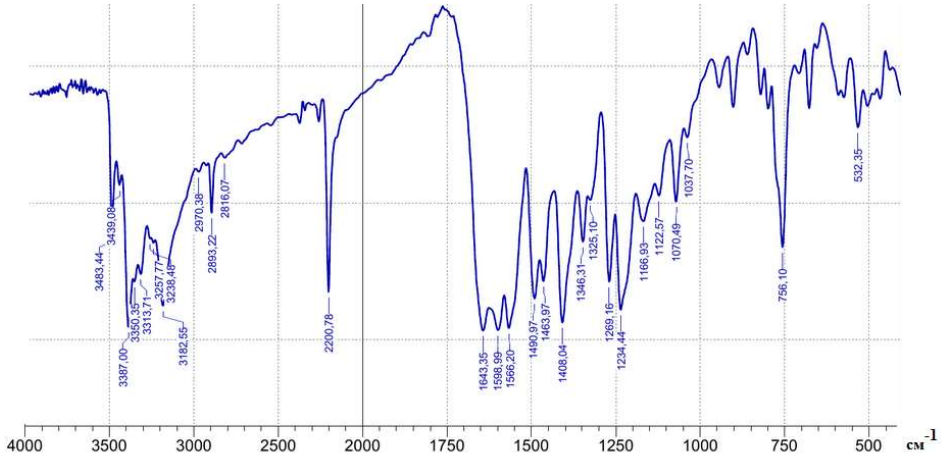
II

Tautomers differ from each other by the place of =NH and –NH2 groups and by the angle the ring R4 is twisted about.

Mostly different geometrical parameters of the tautomers

Bond	Length of the bond, A		Bond	Length of the bond, A	
	(I)	(II)		(I)	(II)
C_5-C_{10}	1,463	1,371	C_5-C_9	1,362	1,467
C_{11}-N_{20}	1,407	1,424	C_9-O_{16}	1,359	1,377
C_9-N_{37}	1,377	-	C_{10}=N_{35}	1,290	-
C_{10}-N_{37}	-	1,387	C_{10}=N_{35}	-	1,281
			Angle		
O_{16}-C_9-C_8	124	117	C_{11}-C_{12}-C_7	110	106

Measured and simulated IR spectra



ν_{exp}, cm^{-1}	ν_{theor}, cm^{-1}		I,km/mol		Assignment	
	I	II	I	II	I	II
1037	-	1054	-	137,6	‡	Q_{R2} (CO), $\beta_{R2\,R6}$ (C=NH), $\beta_{R3\,R6}$ (C=NH)
	1252	-	102,6	-	Q_{R4} (CC), $\beta_{R3\,R6}$ (C=NH), β_{R4} (CCH)	‡
1346	-	1353	-	101,3	‡	β_{R2} (CCH), $\gamma_{R2\,R3}$ (CCCH), γ_{R2} (CCCH), $\gamma_{R1\,R2}$ (CCCH), Q_{R1} (CC), γ_{R3} (HCCH), $\beta_{R1\,R3}$ (CCH)
1346	-	1365	-	209,0	-	γ_{R3R5} (HCCC), $\beta_{R1\,R3}$ (CCH), γ_{R3} (HCCC), $\gamma_{R2\,R3}$ (CCCH), β_{R3} (CCH), $\beta_{R3\,R6}$ (C=NH)
	-	1372	-	24,3	-	Q_{R3} (CN), $\beta_{R3\,R7}$ (CNH), $Q_{R3\,R7}$ (CN), $\beta_{R3\,R6}$ (C=NH), $\gamma_{R3\,R7}$ (CCN)
1597	1590	-	9,1	-	Q_{R1} (CC), β_{R1} (CCH), δ_{R7} (HNH), γ_{R1} (CCC)	‡
	-	1611	-	261,9	-	$Q_{R2\,R6}$ (C=N), Q_{R2} (CC), γ_{R3R2} (CCO)
	1622	-	621,0	-	$Q_{R3\,R6}$ (C=N), $Q_{R3\,R2}$ (CC), δ_{R7} (HNH), $\beta_{R2\,R7}$ (CNH), $Q_{R2\,R7}$ (CN)	‡
	-	1627	-	65,4		δ_{R7} (HNH)
1643	1644	-	64,2	-	$Q_{R3\,R6}$ (C=N), $Q_{R2\,R3}$ (CC), $Q_{R2\,R7}$ (CN)	‡
	-	1644	-	162,0		$Q_{R3\,R6}$ (C=N)
3439 3483	3466	3439	43,4	63,2	q_{R7} (NH)	

CONCLUSIONS

1. **The structure of tautomers I, II was established.**
2. **The presence of tautomers I, II in the sample was established.**
3. **The IR spectrum was interpreted.**
4. **The spectral and structural characteristics of compounds I and II have been established.**
5. **Experimental IR spectrum is superposition of spectra of tautomers I and II.**