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FTIR study of urea and thiourea

Ioana Stanciu*
Faculty of Chemistry, Department of Physical Chemistry, University of Bucharest, Elisabeta Blvd, Bucharest, Romania

Abstract

In this article we have determined by IR spectroscopy the chemical composition of urea and thiourea. The spectrometer used is called IFS Brukker 66v. Both urea and thiourea have bands between 3500 and 750cm^{-1}. They contain the following functional groups: NH stretching, C=O stretching, NH bending, CN assymetric stretching, CN stretching and C=S rocking.

Keywords: Urea, thiourea, FTIR, study

Introduction

Urea (also called carbamide, with the systematic name carbonyl diamide[4]) is an organic compound with the chemical formula $CO(NH_2)_2$. Urea is, in fact, the diamide of carbonic acid, therefore an amide. It is so called because it is obtained from carbonic acid (siphon), by a double reaction of the acid with ammonia [1, 5].

Urea plays an important role in the metabolism of nitrogen compounds in the body of animals, being the main nitrogen compound in the urine of mammals. It is a colorless, crystalline solid, highly soluble in water and practically devoid of toxicity (LD50 is 15 g/kg for rats). At the body level, urea is used in several biochemical processes, the most important being the excretion of nitrogen. It is formed in the liver following the reaction between ammonia (NH_3) and carbon dioxide (CO_2) as part of the urea cycle. The compound is also used as a fertilizer, as a source of nitrogen, and is a very important precursor in the chemical industry.

Thiourea (also called thiocarbamide) is an organic sulfur compound with the formula $SC(NH_2)_2$. It is structurally similar to urea, but the oxygen atom is replaced by a sulfur atom. The properties of thiourea are very different from those of urea. Thiourea is used as a reagent in organic synthesis. The term can also refer to the class of thioureas, which includes compounds with the general structure $(R_1R_2N)(R_3R_4N)C{=}S$. Thioureas are structurally related to thioamides, $RC(S)NR_2$, where R can be methyl, ethyl, etc. radicals [6, 12].

Materials and methods

The FTIR spectral analyses of urea and thiourea have been carried out between 400 and 4000 cm^{-1} on an IFS Brukker 66v spectrometer.

The FTIR spectral data are summarized in Table 1 and the spectra are shown in Figs. 2 and 3. The broad bands around 3362 cm^{-1} and 3455 cm^{-1} ssigned to NH stretching vibration of urea and thiourea. The absorption observed corresponds to the 1454 and 1478 cm^{-1} absorption of urea and thiourea, respectively, and can be assigned to the N–C–N stretching vibration. The broad envelope positioned between 2888 cm-1 of corresponds to asymmetric stretching modes of NH_2 group of thiourea. The absorption at 1785 cm^{-1} is due to C=O stretching of urea. The frequency assigned for NH_2 bending at 1589 cm^{-1}, which shows the presence of urea part of the molecule [13, 17].

Fig 1: IFS Brukker 66v spectrometer

Results and discussions

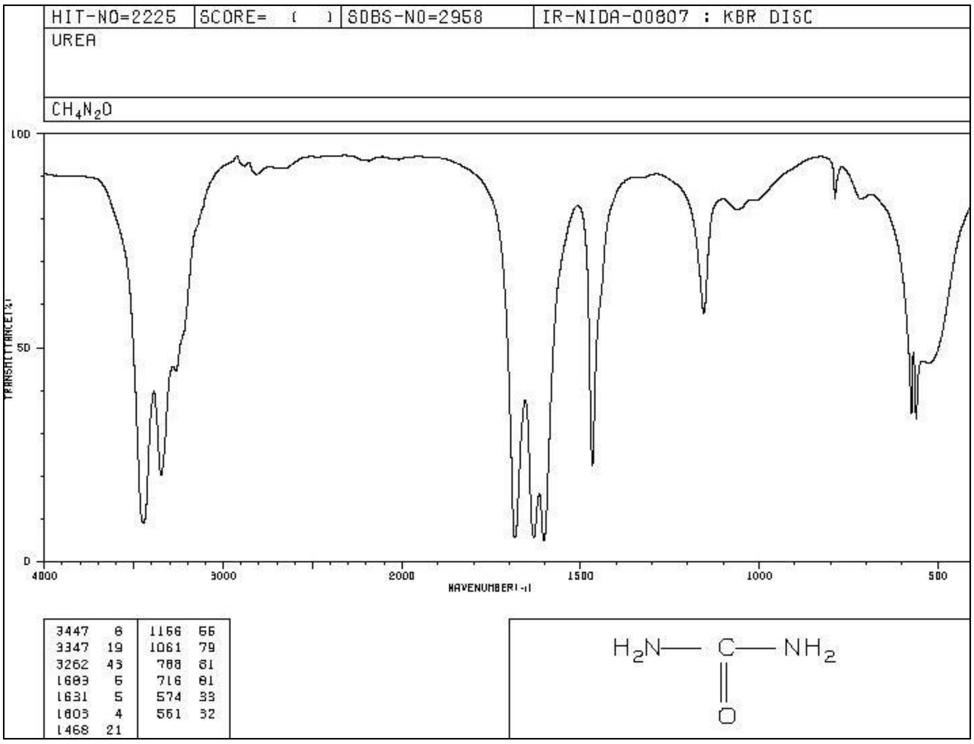

Fig 2: Spectre IR urea

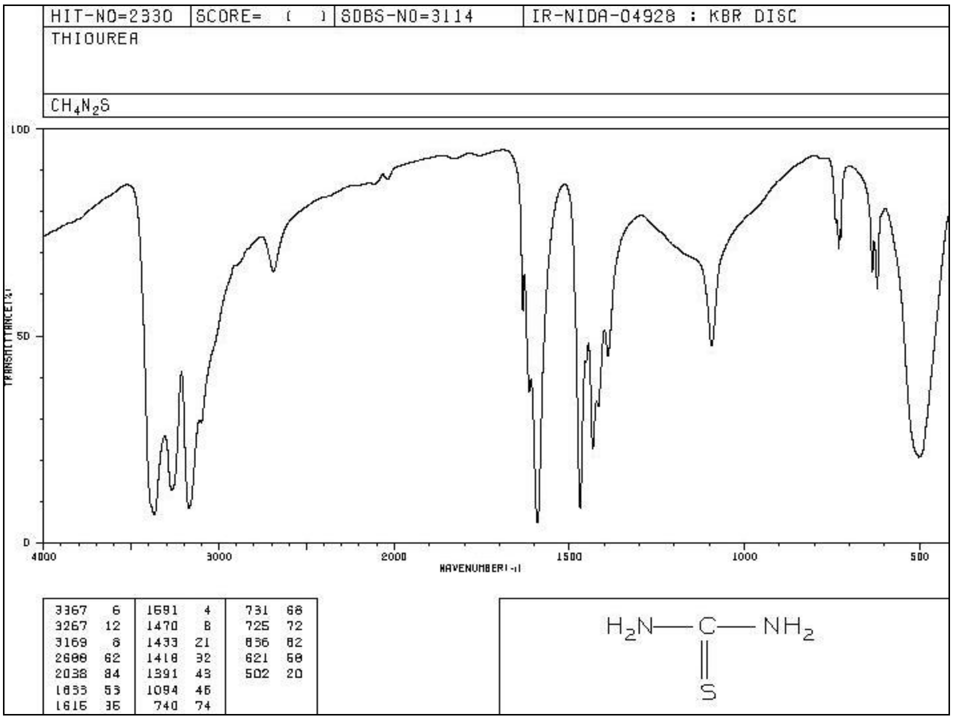

Fig 3: Spectre IR thiourea

Table 1 shows the peak allocation for urea and thiourea.

Table 1: FTIR vibrational frequencies of urea and thiourea

Urea	Thiourea	Assignments
3455	3362	NH stretching
	1671	C=O stretching
1625	1591	NH bending
1454	1478	CN assymetric stretching
1064	1093	CN stretching
	732	C=S rocking

Conclusions

Both urea and thiourea have bands between 3500 and 750cm^{-1}. They contain the following functional groups: NH stretching, C=O stretching, NH bending, CN assymetric stretching, CN stretching and C=S rocking between 3500 and 750cm^{-1} and were determined with the IFS Bruker 66v spectrometer.

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