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Synthesis and Infrared studies on N-(Cyclohexyl)-2-Mercaptoacetamides

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The work describes the IR studies of N-(cyclohexyl)-2-mercaptoacetamides.

INTRODUCTION

N-(Cyclohexyl)-2-mercaptoacetamide was synthesised by the method given by Sircar *et al*[1]. In this synthesis an oxygen free nitrogen atmosphere was used. The purity was checked by T.L.C. and m.p. and the IR spectral studies were made.

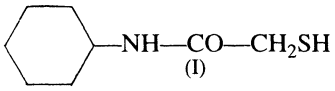
EXPERIMENTAL

Sircar *et al*[1]. method was used in the preparation of N-(cyclohexyl)-2-mercaptoacetamide. The crude product was washed with water to remove any unreacted thioglycolic acid and cyclohexylamine. Finally the compound was dried in *vacuo* (Yield = 7.8 gm and m.p. 73°C). Purity of the above ligands was checked by T.L.C. using iodine as a developer and methanol as a mobile phase and also estimated for nitrogen and mercapto group.

RESULT AND DISCUSSION

IR spectral studies of N-(cyclohexyl)-2-Mercaptoacetamide

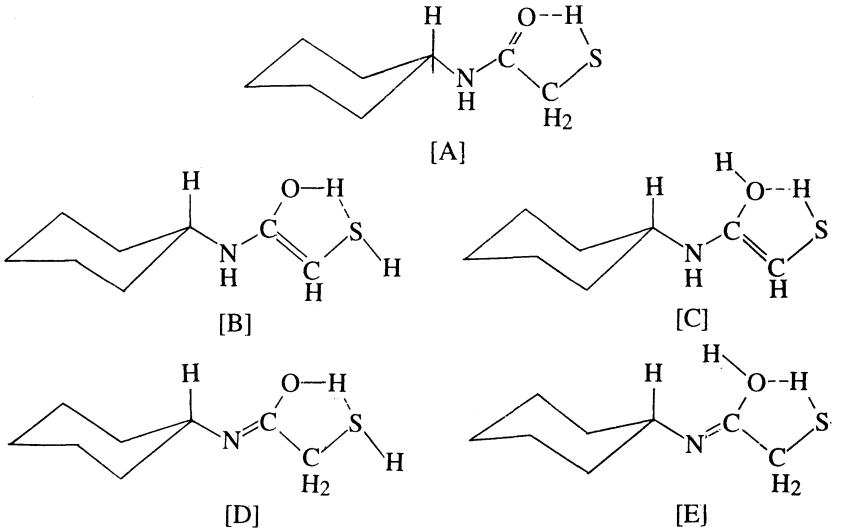
The IR spectrum have been recorded in KBr optics on a double beam Perkin-Elmer 577 infrared spectrophotometer, fitted with a grating. The absorption bands of N-(cyclohexyl)-2-mercaptoacetamide(I) together with assignments are discussed.



(I)

Cyclohexyl moiety is saturated and non-planer (when chair conformation is considered) the mercaptoacetamide group is attached at the axial position of the cyclohexyl ring. A study of the molecular models shows that while merceptoacetamide group staying at the equatorial position there are five possible structures. Out of these five structures C and E are untenable because of the restricted movement of —OH group attached to the carbon. Structure A is ruled out because of the fact that the acidic NH group will tend to pass into another

canonical structure (D). In the structure D the C—OH group is linked to one of the sulphur lone pair of electrons through hydrogen bonding as a consequence of this SH proton ionises more readily than could be anticipated on the basis of structures A, C and E.



The IR spectrum of N-(cyclohexyl)-2-mercaptoacetamide shows two medium to weak intensity bands in region 3270–3240 cm^{-1}. The higher wave number band has been assigned to ν_{as} NH which is of low intensity and the lower wave number band has been assigned to ν_{S-NH}. The lowering in intensity of these two bands are clearly indicative of the tautomeric structure D.

Two bands in the region 2940–2850 cm^{-1} have been observed which have been ascribed to a symmetric and asymmetric C-H stretching vibrations of methyl and methylene groups. These bands are of medium intensity. Likewise two bands in the region 2660–2620 cm^{-1} have been observed which are assigned to asymmetric and symmetric C–H stretching vibrations arising from cyclohexyl group preferentially in the chair form.

The band in the region 2560 cm^{-1} is of medium intensity and this is assigned to stretching vibration of S-H groups. A strong intensity band in the region 1630 cm^{-1} has been assigned to a combination band arising from the coupling of $\nu_{C=O}$ and δ_{NH} vibrations. A broad strong intensity band has been observed in the region 1600–1500 cm^{-1}. This has been ascribed to CH_2 scissors deformation, an asymmetric deformation of CH_2 group. Further two medium intensity bands have been observed in the region 1472–1460 cm^{-1} and these bands have been assigned to a combination bands arising from ν_{N-H} and δ_{C-N}.

On considering the resonating structures on N-(cyclohexyl)-2-mercaptoacetomide (structure D) the ν_{C-O} vibrations are found in the region 1280–1205 cm^{-1}. A series of bands from strong to weak intensity occur in this region. The out-of-plane deformation vibrations of C–H occur in the region 890–842 cm^{-1} likewise, the out-of-plane wagging mode of N –H alongwith C–H

wagging also occur in the region 790–770 cm^{-1}. These bands are of medium tc weak intensity.

From very strong to weak intensity band have been observed in the region 698–507 cm^{-1}originating from ring vibrations. In view of the above discussion structure D is proposed for N-(cyclohexyl)-2-mercaptoacetamide.

REFERENCES

1. R.N. Mishra and S.S. Guha Sircar, *J. Indian Chem. Soc.*, **32**, 127 (1955).

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