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Rao C N R & Venkataraghavan R. The C=S stretching frequency and the "—N—C=S bands" in the infrared. *Spectrochim. Acta* 18:541-7, 1962.

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Assignments are made of the C=S stretching frequency in simple thiocarbonyl compounds and mixed vibrational modes involving this frequency in thioamide-type derivatives. [The SCI® indicates that this paper has been cited in over 215 publications.]

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It is wonderful to hear that this paper has been considered to be useful by so many of my professional colleagues. I wrote this paper when I was a young lecturer in this institute trying hard to build a research career for myself. One of the areas of research that I had decided to work on was chemical spectroscopy (vibrational and electronic). This was difficult to do since there was no spectrometer in the institute. This situation was not easy to reconcile myself to, soon after returning from five years in the US. I then decided to work on problems of sufficient importance that could be investigated with marginal or borrowed facilities. This paper is a result of such an effort.

At the time I wrote this paper, we had no knowledge of the frequency range for the stretching vibration of the C=S group. Unlike the C=O stretching vibration, which was well characterized in a variety of carbonyl derivatives, the characterization of the C=S vibrational frequency in the corresponding organic compounds had been found to be difficult. It was clear that the main problem was the presence of extensive vibrational mixing of the C=S stretching mode with other modes in thioamides, thioureas, and other derivatives. Localized

C=S stretching mode frequencies that would occur in the simplest of thiocarbonyl compounds were not known because of the instability of many of the compounds. We therefore studied the infrared spectra of stable thiocarbonyl compounds exhibiting localized C=S stretching modes. Several of the compounds had to be synthesized. The spectra were recorded by going to laboratories in India that had infrared spectrometers.

Having established the characteristic frequency range of the localized stretching mode, we then examined the infrared spectra of thiomides and such derivatives where the C=S stretching mode is strongly coupled to C—N stretching and other vibration modes. This study gave characteristic frequency ranges of vibrational bands with significant contribution from C=S stretching. The vibrational assignments made by us could be readily used to characterize a variety of thiocarbonyl compounds.¹⁴ The utility of the correlations presented were more useful than I thought at that time.

The situation in my laboratory changed for the better around 1965 when we obtained a spectrometer in my institute. Today, there are many infrared (NMR and other) spectrometers in India, and young people may find it difficult to believe that I published around a dozen or more important papers in vibrational spectroscopy in my early professional years without having a spectrometer in the laboratory.

R. Venkataraghavan, who worked with me on this problem during 1960-1963, was an eager and enthusiastic doctoral student. After his PhD degree with me, he went to Canada and then to the US. He is now a leading worker in mass spectrometry in the US.

It is truly gratifying that a piece of research I carried out as an aspiring spectroscopist when I had no access to an infrared spectrometer has become a *Citation Classic*. This recognition has made me nostalgic about my early experiences as a young research worker.

1. Bellamy L J. *The infra-red spectra of complex molecules*. London: Chapman & Hall, 1975. 433 p.
2. Cornea F, Cercasov C & Clarescu M. Infrared spectra of several thiopiperidides and thiomorpholides. *Spectrochim. Acta* 36A:775-82, 1980.
3. El-Azmy A A & Mostafa M M. Metal chelates of 1-acetylpyridinium chloride-4-phenyl-3-thiosemicarbazide. *Polyhedron* 2:591-3, 1983.
4. Mindl J, Sterba V, Kaderabek V, Jr. & Klícnar I. Kinetics and mechanism of hydrolysis of benzhydryl N-arylothiocarbamates and study of their IR spectra. *Collect. Czech. Chem. Commun.* 49:1577-91, 1984.