

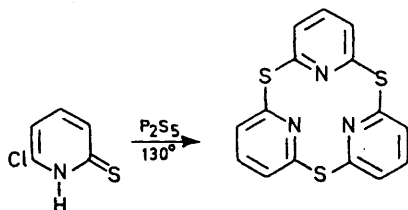
## A New 12-Membered Heterocyclic Ring System

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**Summary** Intermolecular condensations of 6-chloropyridine-2-thione has given a new 12-membered heterocyclic ring system which by X-ray analysis has been found to have a nonplanar conformation.

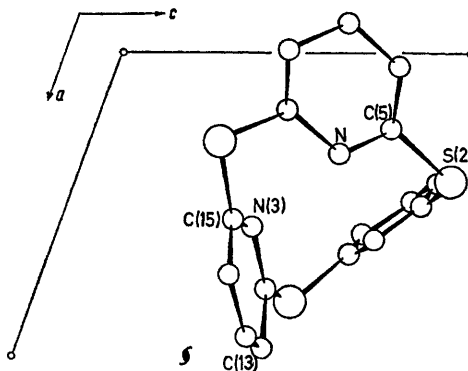
CYCLIC trimers of five-membered mono-heterocycles linked by vinylene bridges have been studied as analogues of [18]annulene.<sup>1</sup> We report initial data from a series of large ring heterocycles where the vinylene bridges between the



heterocyclic monomers, which are part of the macrocyclic ring system, have been replaced by sulphur. The simplest monomer reactant studied was 6-chloropyridine-2-thione.

The crystals were found to be monoclinic with space-group  $P2_1/c$ ;  $a = 14.217$ ,  $b = 7.885$ ,  $c = 15.207$  Å,  $\beta = 119.57^\circ$ ;  $Z = 4$ . The structure was solved by direct methods and refined by full-matrix least-squares  $R$  ca. 2.8% for 1115 reflections recorded on an automatic four circle diffractometer.

The molecule has a pseudo mirror plane through S(2), N(3), and C(13) (Figure). Average bond distances and angles are: C-S: 1.780, C-N: 1.335, C-C: 1.376 Å;  $\angle$  C-S-C: 101.9°, N-C-S: 117.7°, C-C-S: 118.7°, C-N-C: 116.7°,



FIGURE

N-C-C:  $123.5^\circ$ , C-C-C:  $118.6^\circ$  with estimated standard deviations of ca. 0.005 Å and  $0.4^\circ$ . The three angles between the ring planes are  $66^\circ$ ,  $61^\circ$ , and  $57^\circ$ .

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<sup>1</sup> G. M. Badger, G. E. Lewis, and U. P. Singh, *Austral. J. Chem.*, 1966, **19**, 1461 and references therein.