

Short Communications

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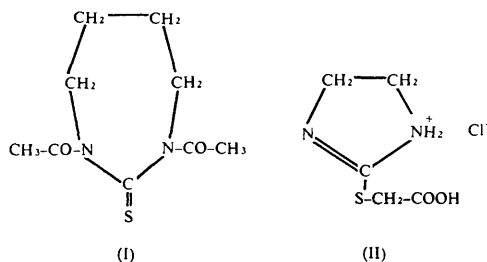
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The unit-cell dimensions and space group of *N,N'*-diacetyl-2-thio-perhydrodiazepine and of imidazoline-2-thioglycollic acid hydrochloride. By G. DEL PIERO and C. DI BELLO, *Institute of Organic Chemistry, 35100 Padova, Italy.*

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Crystals of *N,N'*-diacetyl-2-thio-perhydrodiazepine and of imidazoline-2-thioglycollic acid hydrochloride have been examined by X-rays. They crystallize in the monoclinic system, space group *Ia*, and in the tetragonal system, space group *I4₁/a*, respectively.

In the course of investigations of structures of thioamides, cyclic thioureines and related compounds (Del Pra, 1967; Del Pra, Di Bello & Mammi, 1967; Mammi, Del Pra & Di Bello, 1967; Mammi, D'Angeli & Bezzi, 1965) *N,N'*-diacetyl-2-thio-perhydrodiazepine (I) and the imidazoline-2-thioglycollic acid hydrochloride (II) have been examined by X-rays.



Compound (I) was prepared by acetylation of 2-thio-perhydrodiazepine with acetic anhydride under various conditions (Di Bello, Giormani & D'Angeli, 1967) while compound (II) was obtained by refluxing an aqueous solution of ethylenethiourea with an excess of chloroacetic acid (Johnson & Edens, 1942).

Single crystals of both compounds were grown from ethanol solution as colourless prisms.

From Weissenberg and precession photographs of zero and upper layers the crystal symmetry and the unit-cell dimensions of the two compounds were determined.

The crystal densities were measured by flotation in water-potassium iodide for (I) and in carbon tetrachloride-benzene for (II). All the unit cells chosen proved to be reduced (Buerger, 1957). The physical and crystallographic data are reported in Table 1. No further work is contemplated.

Table 1. *Crystallographic data*

	(I)	(II)
M.W.	C ₉ H ₁₄ O ₂ SN ₂ 214.3	C ₅ H ₈ O ₂ SN ₂ 160.2
m.p. (°C)	106	225
Crystal system	monoclinic	tetragonal
Space group	<i>Ia</i> *	<i>I4₁/a</i>
<i>a</i> (Å)	8.98 ± 0.01	20.82 ± 0.02
<i>b</i> (Å)	11.29 ± 0.01	—
<i>c</i> (Å)	10.53 ± 0.01	7.08 ± 0.01
β (°)	99.4 ± 0.2	—
<i>V</i> (Å ³)	1084	3070
<i>D_x</i> (g.cm ⁻³)	1.31	1.39
<i>D_m</i> (g.cm ⁻³)	1.34	1.37
<i>Z</i>	4	16
<i>F</i> (000) (e)	456	1344
Cu Kα (cm ⁻¹)	18.4	23.2
Mo Kα (cm ⁻¹)	2.1	2.6
Elongation direction	[100]	[001]

The *I2/a* space group has been rejected on the basis of chemical considerations.

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