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N-Chloro-succinimide.

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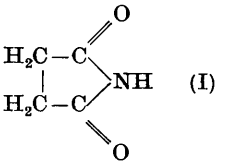
In undertaking a crystallographic investigation of the heterocyclic compound succinimide (I), attention was paid to the parent compound and three of its *N*-halogen derivatives.



(I)

Morphological data on these four compounds were published by Stefl (1915), and Tutton (1925) made an optical and goniometric study of iodo-succinimide. X-ray studies have been made of succinimide and iodo-succinimide (Yardley, 1924, 1925). Information from these sources and from the present work is collected in Table 1.

It was decided to study further the isomorphous chlorine and bromine derivatives by the heavy-atom method. The position of the heavy atom and the approximate molecular orientation were obtained for the bromine compound, and this information was applied to the chlorine isomorph. Refinement has been carried out by two-dimensional Fourier and difference syntheses in the (0*kl*) and (*h*0*l*) zones, for which at present *R* has the values 0·14 and 0·22 respectively.

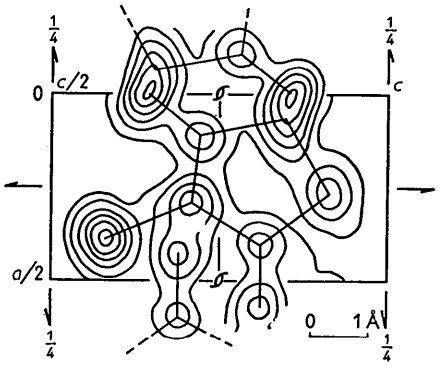


Fig. 1. Early Fourier synthesis down [010]. Contours at approximately 2, 4, 6, ... e.Å^{-2}, except for the chlorine atom, which has contours at 2, 4, 8, 12, 16, ... e.Å^{-2}.

Only a very brief description of the structure will be given here. Fig. 1 shows an early Fourier projection on to the (010) plane, which is that suffering least from atomic overlap. The molecule shown lies almost parallel to the ($\bar{3}73$) plane, and the other three lie at symmetrically related angles. There can be no hydrogen bonding, but there appears to be a rather short Cl–O distance of about 2·9 Å. If this represents a strong intermolecular bond, it will link the molecules in zigzag chains running parallel to [100] at two different levels above the (010) plane.

The molecule appears to be approximately planar. The maximum deviation from the mean plane through the eight heavy atoms is 0·2 Å in the case of the chlorine atom, and, should this be confirmed in the subsequent refinement, it will represent an appreciable distortion of the ideally planar bonding system of the nitrogen atom.

Refinement is proceeding, and a fuller paper will be published later.

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References

Stefl, A. (1915). *Z. Kristallogr.* **54**, 373.
Tutton, A. E. H. (1925). *Proc. Roy. Soc.* A, **108**, 548.
Yardley, K. (1924). *Proc. Roy. Soc.* A, **105**, 462.
Yardley, K. (1925). *Proc. Roy. Soc.* A, **108**, 542.

Table 1. *Crystallographic data*

	Succinimide (Yardley)	Succinimide (this work)	*N*-Chloro-succinimide (this work)	*N*-Bromo-succinimide (this work)	*N*-Iodo-succinimide (Yardley)
a (Å)	7·50	7·51±0·04	6·41±0·01	6·48±0·03	6·29
b (Å)	9·60	9·63±0·05	7·11±0·01	7·25±0·03	—
c (Å)	12·75	12·90±0·06	11·69±0·01	11·86±0·05	15·55
Space group	*Pbca*	*Pbca*	$P2_12_12_1$	$P2_12_12_1$	$P4_1$ or $P4_3$
Density (g.cm.$^{-3}$)	1·419	1·412 (Stefl)	1·650 (Stefl)	2·098 (Stefl)	2·408 (Tutton)
Z	8	8	4	4	4