

dans le cas de la molécule oxygénée, l'angle dièdre O(3)–C(2)–C(1)=O(1) est plus ouvert (39 au lieu de 29°) et que l'angle formé par le noyau benzénique et le plan C(5), O(3), C(2) est plus faible (10 au lieu de 20°). Notons enfin l'ouverture appréciable de l'angle O(3)–C(2)–C(3) (116°), particularité structurale que l'on ne retrouve pas pour d'autres lactones comportant une liaison C–O en  $\alpha$  du carbonyle (Jeffrey, Rosenstein & Vlasse, 1967; Kim, Jeffrey, Rosenstein & Corfield, 1967).

### Références

- BALLY, R., DELETTRE, J. & MORNON, J. P. (1973). *AFFINE*. Laboratoire de Minéralogie–Cristallographie, Univ. de Paris VI, France.
- BENEDETTI, E., GANIS, P., BOMBIERI, G., CAGLIOTI, L. & GERMAIN, G. (1975). *Acta Cryst.* **B31**, 1097–1100.
- BRIANSO, M. C., GALSOMIAS, J., LERE-PORTE, J. P. & PETRISSANS, J. (1980). *Acta Cryst.* **B36**, 2493–2495.
- BRYAN, R. F. & SHEN, M. S. (1978). *Acta Cryst.* **B34**, 327–329.
- DESTRO, R. & COLOMBO, A. (1979). *J. Chem. Soc. Perkin Trans.* 2, pp. 896–899.
- HARLOW, R. L. & SIMONSEN, S. H. (1976). *Acta Cryst.* **B32**, 2137–2144.
- International Tables for X-ray Crystallography* (1974). Tome IV. Birmingham: Kynoch Press.
- JEFFREY, G. A., ROSENSTEIN, R. D. & VLASSE, M. (1967). *Acta Cryst.* **22**, 725–732.
- KIM, S. H., JEFFREY, G. A., ROSENSTEIN, R. D. & CORFIELD, P. W. R. (1967). *Acta Cryst.* **22**, 733–743.
- KOK, P., DE CLERCQ, P., VANDEWALLE, M., DECLERCQ, J. P., GERMAIN, G. & VAN MEERSSCHE, M. (1979). *Tetrahedron Lett.* **22**, 2063–2066.
- LERE-PORTE, J. P., GALSOMIAS, J. & PETRISSANS, J. (1979). Réunion de la section méditerranéenne de la Société de Chimie Physique, Barcelone.
- MAIN, P., LESSINGER, L., WOLFSON, M. M., GERMAIN, G. & DECLERCQ, J. P. (1977). *MULTAN 77. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. de York, Angleterre, et Louvain-la-Neuve, Belgique.
- MERLINO, S. (1971). *Acta Cryst.* **B27**, 2491–2492.
- THIESSEN, W. E. & HOPE, H. (1970). *Acta Cryst.* **B26**, 554–562.

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## Structure of Xanthomegnin

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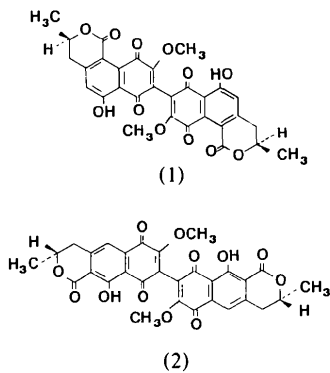
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**Abstract.** C<sub>30</sub>H<sub>22</sub>O<sub>12</sub>,  $M_r = 574.49$ , tetragonal,  $P4_32_12$ ,  $a = 8.126$  (1),  $c = 38.281$  (4) Å,  $Z = 4$ ,  $D_m = 1.50$  (2) (floatation),  $D_x = 1.510$  Mg m<sup>-3</sup>,  $\mu(\text{Cu } K\alpha) = 0.958$  mm<sup>-1</sup>;  $R = 0.034$  for 1270 observed reflections. X-ray analysis has revealed that xanthomegnin is a naphtho-[2,3-*c*]pyran-8-yl dimer. A crystallographic twofold axis relates the two halves of the molecule. In each half of the molecule there is one intramolecular hydrogen bond.

\* From a dissertation to be submitted to the Graduate School, The Catholic University of America, Washington, DC 20064, in partial fulfillment of the requirements for the PhD degree in chemistry.

**Introduction.** Xanthomegnin, a metabolite of pathogenic fungi, was first isolated from *Trichophyton megnini* and was assigned the dimeric structure (1) on the basis of degradation studies and chemical and spectroscopic evidence (Just, Day & Blank, 1963; Ng, Just & Blank, 1969). Xanthomegnin has also been isolated from *T. violaceum* (Ng, Just & Blank, 1969), *T. rubrum* (Wirth, Beesley & Anand, 1965), *Microsporum cookei* (Ito, Kawai & Nozawa, 1973), *Aspergillus sulphureus*, *A. melleus* (Durley, MacMillan, Simpson, Glen & Turner, 1975; Simpson, 1977), *A. ochraceus*, *Penicillium cyclopium* and *P. viridicatum* (Stack & Mislivec, 1978; Stack, Eppley, Dreifuss & Pohland, 1977). Subsequent studies of xanthomegnin

and related compounds provided additional spectral and chemical data which were reported to be consistent with the original structural assignment (Durley, MacMillan, Simpson, Glen & Turner, 1975; Simpson, 1977). Alternate structure (2) has recently been proposed based on the  $^{13}\text{C}$  NMR spectra of xanthomegnin and xanthomegnin diacetate in which only minor differences from the previously reported spectra were observed (Höfle & Röser, 1978). Thus, the X-ray structure determination of xanthomegnin was undertaken to resolve the ambiguity in the literature regarding the orientation of the lactone ring. This structure analysis reveals the molecular configuration for xanthomegnin (2) and provides an accurate basis for establishing the ring structures of closely related metabolites isolated from *P. viridicatum*, including viomellein, rubrosulphin, viopurpurin, xanthoviridicatin D and xanthoviridicatin G (Stack, Mazzola & Eppley, 1979).



For this X-ray work, (2) was isolated from *P. viridicatum* by procedures described in the literature (Stack & Mislivec, 1978; Stack, Eppley, Dreifuss & Pohland, 1977). Red-orange crystals suitable for single-crystal X-ray analysis were obtained by recrystallization from acetonitrile. Data were collected on a crystal of dimensions  $0.20 \times 0.28 \times 0.36$  mm using an automated four-circle diffractometer with graphite-monochromated  $\text{Cu K}\alpha$  radiation,  $\lambda = 1.54178$  Å. Cell dimensions were determined by a least-squares refinement of the setting angles of 15 reflections with  $2\theta$  values ranging between 61 and  $94^\circ$ . Systematic extinctions observed on the diffractometer established the space group as  $P4_12_12$  or its enantiomorph  $P4_32_12$ ; the latter was chosen because it requires an  $R$  configuration of the asymmetric center in the lactone ring. This is consistent with the absolute stereochemistry previously established by degradation of (2) to  $(-)$ - $(R)$ - $\beta$ -hydroxybutyric acid (Ng, Just & Blank, 1969). Integrated diffraction intensities were measured in the range  $4.0 \leq 2\theta \leq 150.0^\circ$ . The peaks were scanned from  $2\theta(K\alpha_1) - 0.8^\circ$  to  $2\theta(K\alpha_2) + 1.1^\circ$  for  $4.0 \leq 2\theta \leq 115.0^\circ$  and  $2\theta(K\alpha_1) - 0.9^\circ$  to  $2\theta(K\alpha_2) + 1.9^\circ$  for  $115.0 \leq 2\theta \leq 150.0^\circ$ . Variable scan rates of

$2.0$  to  $29.3^\circ \text{ min}^{-1}$  were used depending on the intensity of the preliminary count. Background counts were taken at each end of the scan with a ratio of total background time to scan time of 0.5. Four standard reflections which were measured periodically showed no apparent decrease in intensity during data collection. The estimated standard deviation in intensity,  $\sigma(I)$ , was calculated from  $\sigma^2(I) = \text{TC} + 0.000198\text{TC}^2$  where TC is the total observed counts and the constant was derived from a statistical analysis of the intensity distributions of the four standard reflections. The data were corrected for Lorentz and polarization effects. Absorption corrections were applied using the Gaussian quadrature method. Of the 1365 unique reflections measured, 1270 had  $I \geq 3\sigma(I)$  and were subsequently used for structure determination and refinement.

The structure was solved by direct methods using *MULTAN* (Germain, Main & Woolfson, 1971) and was refined by full-matrix least-squares calculations.

Table 1. Positional parameters and isotropic thermal parameters ( $\text{\AA}^2$ ) with estimated standard deviations in parentheses

Equivalent isotropic temperature factors for the nonhydrogen atoms were calculated from  $U_{\text{eq}} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$ . Coordinates of the atoms in the second half of the molecule may be calculated from  $1 - y$ ,  $1 - x$ ,  $-\frac{1}{2} - z$ .

|        | <i>x</i>   | <i>y</i>   | <i>z</i>     | $U_{\text{eq}}/U$ |
|--------|------------|------------|--------------|-------------------|
| C(1)   | 0.6819 (4) | 0.5663 (4) | -0.40682 (8) | 0.067 (2)         |
| C(2)   | 0.7894 (3) | 0.4984 (3) | -0.37877 (7) | 0.0527 (15)       |
| C(3)   | 0.7206 (3) | 0.4163 (3) | -0.34969 (7) | 0.0495 (14)       |
| C(4)   | 0.8241 (3) | 0.3516 (3) | -0.32377 (6) | 0.0437 (13)       |
| C(5)   | 0.7563 (3) | 0.2732 (3) | -0.29283 (7) | 0.0462 (13)       |
| C(6)   | 0.8661 (3) | 0.2111 (3) | -0.26554 (6) | 0.0432 (13)       |
| C(7)   | 1.0293 (3) | 0.2203 (3) | -0.26892 (6) | 0.0489 (14)       |
| C(8)   | 1.1063 (3) | 0.2976 (3) | -0.30027 (7) | 0.055 (2)         |
| C(9)   | 0.9952 (3) | 0.3656 (3) | -0.32767 (6) | 0.0463 (14)       |
| C(10)  | 1.0634 (3) | 0.4432 (3) | -0.35618 (7) | 0.057 (2)         |
| C(11)  | 0.9603 (3) | 0.5092 (3) | -0.38173 (7) | 0.055 (2)         |
| C(12)  | 1.0311 (5) | 0.5945 (4) | -0.41313 (8) | 0.069 (2)         |
| C(13)  | 0.9207 (4) | 0.7338 (4) | -0.42395 (8) | 0.069 (2)         |
| C(14)  | 0.9700 (6) | 0.8142 (4) | -0.45805 (8) | 0.088 (3)         |
| C(15)  | 1.2731 (5) | 0.0878 (4) | -0.24525 (8) | 0.084 (2)         |
| O(1)   | 0.7537 (3) | 0.6720 (2) | -0.42941 (5) | 0.0743 (14)       |
| O(2)   | 0.5402 (3) | 0.5327 (3) | -0.41130 (6) | 0.091 (2)         |
| O(3)   | 0.5558 (2) | 0.4022 (2) | -0.34733 (5) | 0.0629 (12)       |
| O(4)   | 0.6053 (2) | 0.2553 (2) | -0.28869 (5) | 0.0650 (12)       |
| O(5)   | 1.1209 (2) | 0.1716 (3) | -0.24167 (5) | 0.0775 (14)       |
| O(6)   | 1.2547 (2) | 0.3082 (3) | -0.30296 (5) | 0.088 (2)         |
| H(O3)  | 0.546 (4)  | 0.354 (3)  | -0.3259 (6)  | 0.100             |
| H(10)  | 1.193 (3)  | 0.461 (3)  | -0.3577 (6)  | 0.076 (9)         |
| H(121) | 1.021 (3)  | 0.523 (3)  | -0.4342 (6)  | 0.094 (11)        |
| H(122) | 1.154 (3)  | 0.636 (3)  | -0.4075 (5)  | 0.070 (9)         |
| H(13)  | 0.909 (3)  | 0.829 (3)  | -0.4037 (6)  | 0.092 (10)        |
| H(141) | 0.971 (4)  | 0.721 (3)  | -0.4751 (7)  | 0.110             |
| H(142) | 0.902 (4)  | 0.907 (3)  | -0.4651 (7)  | 0.110             |
| H(143) | 1.092 (3)  | 0.867 (4)  | -0.4577 (7)  | 0.110             |
| H(151) | 1.248 (4)  | 0.006 (4)  | -0.2631 (7)  | 0.110             |
| H(152) | 1.375 (3)  | 0.181 (3)  | -0.2546 (7)  | 0.110             |
| H(153) | 1.280 (4)  | 0.036 (3)  | -0.2221 (7)  | 0.110             |

All H atoms were located in a difference Fourier map calculated at an intermediate stage of refinement. Anisotropic refinement of the nonhydrogen atoms and isotropic refinement of the H atoms (with the methyl and hydroxy H atoms assigned fixed thermal parameters) resulted in a final  $R$  ( $=\sum ||F_o| - |F_c|| / \sum |F_o|$ ) of 0.034. The function minimized was  $\sum w(|F_o| - |F_c|)^2$  where  $w = [\sigma(F_o)]^{-2}$ . The average and maximum shift divided by error were 0.047 and 0.622, respectively. Analysis of the final difference Fourier map revealed no peak greater than  $0.16 \text{ e } \text{Å}^{-3}$ . The scattering factors used were those of Cromer & Mann (1968) for C and O and that of Stewart, Davidson & Simpson (1965) for H. All calculations (except *MULTAN*) were performed with the XRAY system (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). Table 1\* lists the final atomic parameters.

**Discussion.** The molecular structure for (2) is shown in Fig. 1 which includes the labeling scheme. Selected bond distances and angles are given in Table 2. A crystallographic twofold axis passing through the

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36109 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Bond distances (Å) and angles (°) with estimated standard deviations in parentheses

|                 |           |                   |           |
|-----------------|-----------|-------------------|-----------|
| C(1)–C(2)       | 1.491 (4) | C(6)–C(7)         | 1.335 (3) |
| C(1)–O(1)       | 1.351 (4) | C(7)–C(8)         | 1.492 (4) |
| C(1)–O(2)       | 1.195 (4) | C(7)–O(5)         | 1.341 (3) |
| C(2)–C(3)       | 1.413 (4) | C(8)–C(9)         | 1.491 (4) |
| C(2)–C(11)      | 1.396 (4) | C(8)–O(6)         | 1.213 (3) |
| C(3)–C(4)       | 1.403 (3) | C(9)–C(10)        | 1.376 (4) |
| C(3)–O(3)       | 1.347 (3) | C(10)–C(11)       | 1.395 (4) |
| C(4)–C(5)       | 1.453 (3) | C(11)–C(12)       | 1.502 (4) |
| C(4)–C(9)       | 1.402 (3) | C(12)–C(13)       | 1.503 (5) |
| C(5)–C(6)       | 1.464 (3) | C(13)–C(14)       | 1.514 (5) |
| C(5)–O(4)       | 1.246 (3) | C(13)–O(1)        | 1.461 (4) |
| C(6)–C(6')      | 1.484 (3) | C(15)–O(5)        | 1.419 (4) |
| C(2)–C(1)–O(1)  | 116.3 (3) | C(6)–C(7)–O(5)    | 117.3 (2) |
| C(2)–C(1)–O(2)  | 125.7 (3) | C(8)–C(7)–O(5)    | 121.1 (2) |
| O(1)–C(1)–O(2)  | 118.0 (3) | C(7)–C(8)–C(9)    | 117.9 (2) |
| C(1)–C(2)–C(3)  | 120.7 (2) | C(7)–C(8)–O(6)    | 121.0 (2) |
| C(1)–C(2)–C(11) | 120.1 (2) | C(9)–C(8)–O(6)    | 121.0 (2) |
| C(3)–C(2)–C(11) | 119.2 (2) | C(4)–C(9)–C(8)    | 119.7 (2) |
| C(2)–C(3)–C(4)  | 119.8 (2) | C(4)–C(9)–C(10)   | 121.4 (2) |
| C(2)–C(3)–O(3)  | 119.1 (2) | C(8)–C(9)–C(10)   | 118.9 (2) |
| C(4)–C(3)–O(3)  | 121.1 (2) | C(9)–C(10)–C(11)  | 119.3 (2) |
| C(3)–C(4)–C(5)  | 120.8 (2) | C(2)–C(11)–C(10)  | 121.1 (2) |
| C(3)–C(4)–C(9)  | 119.2 (2) | C(2)–C(11)–C(12)  | 118.4 (2) |
| C(5)–C(4)–C(9)  | 119.9 (2) | C(10)–C(11)–C(12) | 120.6 (3) |
| C(4)–C(5)–C(6)  | 120.1 (2) | C(11)–C(12)–C(13) | 109.8 (3) |
| C(4)–C(5)–O(4)  | 121.9 (2) | C(12)–C(13)–C(14) | 113.9 (3) |
| C(6)–C(5)–O(4)  | 118.0 (2) | C(12)–C(13)–O(1)  | 109.6 (2) |
| C(5)–C(6)–C(7)  | 121.2 (2) | C(14)–C(13)–O(1)  | 105.7 (3) |
| C(5)–C(6)–C(6') | 117.4 (2) | C(1)–O(1)–C(13)   | 121.9 (2) |
| C(7)–C(6)–C(6') | 121.4 (2) | C(7)–O(5)–C(15)   | 123.4 (2) |
| C(6)–C(7)–C(8)  | 121.2 (2) |                   |           |

center of the C(6)–C(6') bond relates the two halves of the molecule. A least-squares-plane calculation through the atoms C(2), C(3), . . . C(11), O(4), O(6) shows that the three-ring system is approximately planar [average deviation =  $0.018 \text{ Å}$ , maximum deviation =  $0.043 \text{ Å}$  for C(6)]. The distances of the remaining atoms from the plane are: O(1),  $0.338 (2)$ ; O(2),  $-0.288 (2)$ ; O(3),  $-0.046 (2)$ ; O(5),  $0.158 (2)$ ; C(1),  $0.011 (3)$ ; C(12),  $0.039 (4)$ ; C(13),  $0.851 (3)$ ; C(14),  $0.790 (4)$ ; C(15),  $-0.530 (4) \text{ Å}$ . The normals to the planes of the two three-ring systems form an angle of  $78.8^\circ$ . In each half of the molecule, there is one intramolecular hydrogen bond between O(3) and O(4) with  $O(3)–H(O3) = 0.91 (2)$ ,  $H(O3)–O(4) = 1.70 (3) \text{ Å}$  and  $O(3)–H(O3)–O(4) = 158 (3)^\circ$ .

The molecular packing is illustrated in Fig. 2. There are no intermolecular contacts significantly shorter than the sum of the van der Waals radii and there is no evidence for intermolecular hydrogen bonding.

The crystal structure of (2) is similar to that of floccosin (Brisse, Just & Blank, 1978), the main pigment of *Epidermophyton floccosum*, in that both are

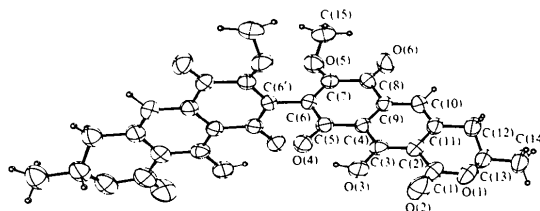


Fig. 1. Molecular structure of xanthomegnin showing the labeling scheme used (ORTEP, Johnson, 1965). The primed atom is related to the corresponding unprimed one by a crystallographic twofold axis (in the plane of the page) passing through the molecule.

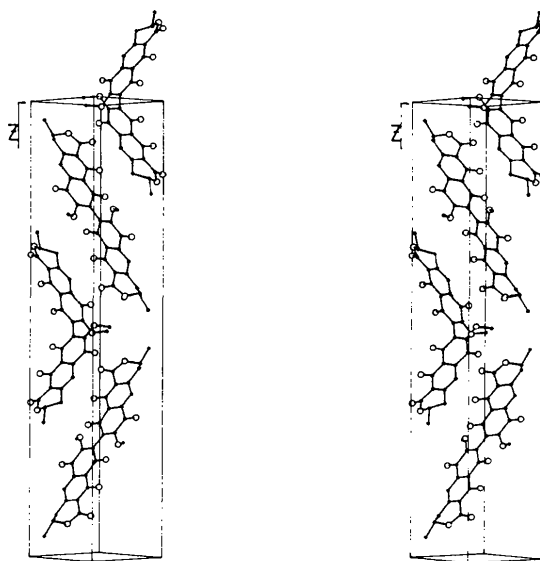


Fig. 2. Stereoscopic view of the packing.

dimers which crystallize in the space group  $P4_32_12$  with  $Z = 4$ . In addition, the molecules of (2) and floccosin resemble each other with respect to the orientation of the two nearly planar three-ring systems. The interatomic distances and angles found for xanthomegnin agree with comparable values reported for floccosin.

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#### References

- BRISSE, F., JUST, G. & BLANK, F. (1978). *Acta Cryst.* **B34**, 557–562.
- CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* **A24**, 321–324.
- DURLEY, R. C., MACMILLAN, J., SIMPSON, T. J., GLEN, A. T. & TURNER, W. B. (1975). *J. Chem. Soc. Perkin Trans.* **1**, pp. 163–169.
- GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* **A27**, 368–376.
- HÖFLE, G. & RÖSER, K. (1978). *J. Chem. Soc. Chem. Commun.* pp. 611–612.
- ITO, Y., KAWAI, K. & NOZAWA, Y. (1973). *J. Biochem.* **74**, 805–810.
- JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.
- JUST, G., DAY, W. C. & BLANK, F. (1963). *Can. J. Chem.* **41**, 74–79.
- NG, A. S., JUST, G. & BLANK, F. (1969). *Can. J. Chem.* **47**, 1223–1227.
- SIMPSON, T. J. (1977). *J. Chem. Soc. Perkin Trans.* **1**, pp. 592–595.
- STACK, M. E., EPPLEY, R. M., DREIFUSS, P. A. & POHLAND, A. E. (1977). *Appl. Environ. Microbiol.* **33**(2), 351–355.
- STACK, M. E., MAZZOLA, E. P. & EPPLEY, R. M. (1979). *Tetrahedron Lett.* pp. 4989–4992.
- STACK, M. E. & MISLIVEC, P. B. (1978). *Appl. Environ. Microbiol.* **36**(4), 552–554.
- STEWART, J. M., MACHIN, P. A., DICKINSON, C., AMMON, H. L., HECK, H. & FLACK, H. (1976). The XRAY system – version of March 1976. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.
- WIRTH, J. C., BEESLEY, T. E. & ANAND, S. R. (1965). *Phytochemistry*, **4**, 505–509.

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## 5-[(*p*-Chlorobenzamido)methylene]-1,3-dimethyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione

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**Abstract.**  $C_{14}H_{12}ClN_3O_4$ , monoclinic,  $P2_1/c$ ,  $a = 15.5124$  (11),  $b = 7.2375$  (3),  $c = 13.3737$  (10) Å,  $\beta = 108.69$  (1)°,  $V = 1422.3$  (2) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.495$  Mg m<sup>-3</sup>,  $M_r = 321.72$ ,  $\mu(\text{Cu } K\alpha) = 2.59$  mm<sup>-1</sup>. The structure was solved by Patterson and Fourier techniques.  $R$  and  $R_w$  were 0.059 and 0.084 respectively for 2038 observed reflexions. The Cl–C(benzene) distance and the *ipso* angle are 1.741 (2) Å and 122.0 (3)° respectively. There is an intramolecular hydrogen bond [N–H...O = 149 (4)°].

**Introduction.** The title compound is the by-product of a reaction which took place when acylation of the C(5) atom in the nucleus of a pyrimidine was attempted. The structure determination was carried out in order to establish the structural formula (Fig. 1).

Unit-cell dimensions were obtained and refined by a least-squares procedure from the setting angles of 78 reflexions with  $\theta \leq 45^\circ$ . The data were collected on a four-circle diffractometer in the  $\omega/2\theta$  scan mode. Graphite-monochromatized Cu  $K\alpha$  radiation was used. 2419 independent reflexions were recorded, 2038 of which were considered as observed [ $I > 2\sigma(I)$ ]. An

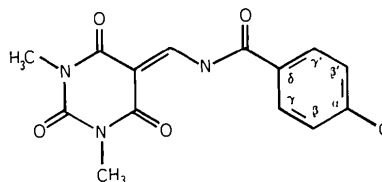


Fig. 1. Structural formula of the title compound.