Fig. 2. The overlapping mode of the two molecules around the inversion center $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$: (a) projection along the normal to the mean plane of the acylurea moiety and (b) side view. Several contacts (Å) are given.

The acylurea moiety, $-$NHCONHCO$-$, is planar within ± 0.017 Å, the intramolecular hydrogen bond N(10)$-$H(10)$\cdots$O(15) being formed. The N(10)$\cdots$ O(15) and H(10)$\cdots$O(15) distances are 2·681 (3) and 1·96 (2) Å, respectively. The mean plane of the acyl-urea moiety makes an angle of 4·26 (8)° with the benzene ring of the p-dimethylaminophenyl group. The methyl groups deviate significantly from the mean plane of the benzene ring in the p-dimethylaminophenyl

group. The plane composed of C(1), C(2) and N(3) makes an angle of 23·5 (3)° with the benzene ring. Bond lengths and angles are given in Table 2. Five $C(sp^2)-$N distances, C(4)$-$N(3), C(7)$-$N(10), C(11)$-$N(10), C(11)$-$N(13) and C(14)$-$N(13), are significantly different from each other; they range from 1·338 to 1·416 Å.

The acylurea moiety and the benzene ring of the p-dimethylaminophenyl group overlap each other as shown in Fig. 2, in which several short contacts between the two moieties are given. The distance between the mean planes of the acylurea moieties is 3·392 (3) Å. Since the present complex is colorless in an acetonitrile solution, the color of the crystal may be brought about by the weak charge-transfer interaction between the acylurea and p-dimethylaminophenyl groups in the crystalline field.

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Structure of 1-(p-Dimethylaminophenyl)-3-(phenylacetyl)urea, C$_{17}$H$_{19}$N$_3$O$_2$

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Abstract. $M_r = 297 \cdot 4$, monoclinic, $P2_1/a$, $a = 12 \cdot 878$ (1), $b = 9 \cdot 954$ (1), $c = 12 \cdot 245$ (1) Å, $\beta = 94 \cdot 92$ (1)°, $V = 1563 \cdot 8$ (3) Å^3, $D_m = 1 \cdot 26$, $D_x = 1 \cdot 265$ g cm^{-3}, $Z = 4$, $T = 293$ K, $F(000) = 148$, μ(Cu $K\alpha$) = 8·02 cm^{-1}, $\lambda = 1 \cdot 54184$ Å, $R = 0 \cdot 049$ for 2160 observed reflections. The benzyl group is approximately at right angles to the remaining part of the molecule. The molecules form a symmetrical dimer structure linked by two N$-$H$\cdots$O hydrogen bonds. The p-dimethylaminophenyl groups in the two molecules around another inversion center are stacked and the dimethylamino group of one molecule is capped by the benzyl group of the other.

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Introduction. The selectivity in the oxidation of a pair of thiols, $HSCH_2(CONH)_2C_6H_4N(CH_3)_2$ (1) and $HSCH_2CH_2(NHCO)_2-R$ (R = alkyl) (2), has been found to depend on the weak interactions between the $C_6H_4N(CH_3)_2$ and R groups (Endo, Kuwahara, Tasai, Murata, Hashimoto & Ishigami, 1977; Endo, Takeda, Orii, Kaneko & Kondo, 1979; Endo, Takeda, Kamada, Kayama & Tasai, 1980; Endo, Takeda, Orii, Murata, Sakai, Nakagawa & Nikki, 1980; Endo, Takeda, Orii, Kuwahara, Ohta, Sakai, Okada & Hashimoto, 1980; Endo, Okubo, Kaneko, Uehara, Tasai, Sato, Nikki, Nakagawa & Kamei, 1982). The structure of (1) was

reported in the previous paper (Uchida, Ohashi, Sasada, Kaneko & Endo, 1984). Since it was very difficult to obtain a crystal of the molecular complex composed of (1) and (2), a series of model compounds such as $R-(CONH)_2C_6H_4N(CH_3)_2$ were prepared, which contained both moieties $C_6H_4N(CH_3)_2$ and R in one molecule. The present work was undertaken to examine the intermolecular interaction between the two groups, $C_6H_4N(CH_3)_2$ and $CH_2C_6H_5$, in the crystal structure.

Experimental. Colorless prismatic crystals obtained from an acetonitrile solution, density measured by flotation in n-C_6H_{12}/CCl_4; systematic absences $h0l$: $h = 2n + 1$, $0k0$: $k = 2n + 1$; approximate dimensions of crystal $0.5 \times 0.3 \times 0.2$ mm, Rigaku AFC-4 diffractometer, graphite monochromator; cell parameters refined by least-squares method on the basis of 20 independent 2θ values, Cu $K\alpha$ radiation ($19° < 2\theta < 27°$); intensity measurement performed up to $2\theta = 120°$ ($\pm h + k + l$ set), θ–2θ scan technique, scan speed $4°$ min$^{-1}(\theta)$; 2321 reflections measured, 2160 intensities with $|F_o| > 3\sigma(|F_o|)$ considered as observed and used for the structure determination; corrections for Lorentz and polarization, absorption ignored; direct methods (MULTAN78, Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); block-diagonal least squares (HBLS, Ohashi, 1975) with anisotropic thermal parameters for all non-H atoms, H atoms located on difference map, $\sum w(|F_o| - |F_c|)^2$ minimized, $w = [\sigma^2(|F_o|) + (C|F_o|)^2]^{-1}$, $C(= 0.015)$ adjusted so that constant values of $\langle w(|F_o| - |F_c|)^2\rangle$ were obtained in the different $|F_o|$ and $\sin\theta$ intervals; final $R = 0.049$, $R_w = 0.058$ for 2160 observed reflections; $(\Delta/\sigma)_{max} = 0.2$; difference-map excursions <0.2 e Å^{-3}; atomic scattering factors from International Tables for X-ray Crystallography (1974); no correction for secondary extinction; calculations carried out on the FACOM–HITAC system M-180 computer at this Institute.

Table 1. *Final atomic coordinates ($\times 10^4$) with their estimated standard deviations and equivalent isotropic thermal parameters*

$$B_{eq} = \tfrac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

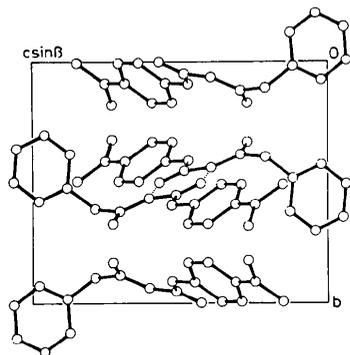|	x	y	z	B_{eq} (Å²)
C(1)	−1655 (1)	3220 (2)	7311 (2)	6·4
C(2)	−768 (2)	4934 (3)	8484 (2)	6·8
N(3)	−788 (1)	4105 (2)	7539 (1)	6·1
C(4)	28 (1)	4116 (2)	6872 (1)	3·9
C(5)	1 (1)	3311 (2)	5942 (1)	4·7
C(6)	806 (1)	3317 (2)	5270 (1)	4·1
C(7)	1667 (1)	4120 (2)	5491 (1)	3·4
C(8)	1708 (1)	4941 (2)	6403 (1)	4·1
C(9)	903 (1)	4931 (2)	7081 (1)	4·2
N(10)	2432 (1)	4082 (1)	4721 (1)	3·9
C(11)	3417 (1)	4503 (2)	4861 (1)	3·4
O(12)	3844 (1)	4984 (1)	5706 (1)	4·3
N(13)	4000 (1)	4364 (2)	3947 (1)	3·7
C(14)	3703 (1)	3823 (2)	2947 (1)	3·9
O(15)	2949 (1)	3311 (1)	2720 (1)	4·9
C(16)	4501 (1)	3927 (2)	2114 (1)	4·4
C(17)	4081 (1)	4808 (2)	1172 (1)	3·5
C(18)	3630 (1)	4252 (2)	219 (1)	4·3
C(19)	3219 (1)	5050 (2)	−631 (1)	5·7
C(20)	3246 (2)	6419 (2)	−534 (2)	6·5
C(21)	3693 (2)	6985 (2)	414 (2)	6·3
C(22)	4113 (1)	6194 (2)	1266 (2)	4·8

Fig. 1. The crystal structure viewed along the a axis. The hydrogen bonds are indicated by dotted lines. H atoms are omitted for clarity.

Discussion. The final atomic parameters for non-H atoms are in Table 1.* The crystal structure viewed along the a axis is shown in Fig. 1. Two molecules around the inversion center ($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) are linked by two N(13)—H(13)$\cdots$O(12) hydrogen bonds to form a dimer, the N(13)$\cdots$O(12) and H(13)$\cdots$O(12) distances being 2·848 (2) and 1·88 (2) Å, respectively. Such a hydrogen-bonded dimer is also found in the crystal of the SH derivative (1). Two molecules around another inversion center, ($0,\frac{1}{2},\frac{1}{2}$), are stacked as shown in Fig. 2.

The acylurea moiety is less planar than that of (1). The mean plane composed of N(10), C(11), O(12) and N(13) makes an angle of 5·37 (7)° with that of N(13), C(14), O(15) and C(16). The intramolecular hydrogen-bond distances N(10)···O(15) and H(10)···O(15) are 2·665 (2) and 1·87 (2) Å, respectively. The mean plane of the acylurea moiety makes angles of 17·06 (5) and 81·65 (6)° with the benzene rings of the *p*-dimethylaminophenyl and benzyl groups, respectively. Bond lengths and angles are given in Table 2. The corresponding values in the present molecule and the SH derivative are in good agreement with each other.

The extent of overlap is smaller than that in the SH derivative. The distance between the mean planes of the benzene rings of the two *p*-dimethylaminophenyl groups is 3·640 (8) Å. The two methyl groups of the *p*-dimethylaminophenyl group are capped by the benzyl group in the other molecule, although the inter-molecular distances between the two groups are not unusually short. Such a mode of approach of the *p*-dimethylaminophenyl and benzyl groups may closely correlate with the shape-specific interaction in the oxidation of a pair of thiols (Endo, Okubo, Kaneko, Uehara, Tasai, Sato, Nikki, Nakagawa & Kamei, 1982).
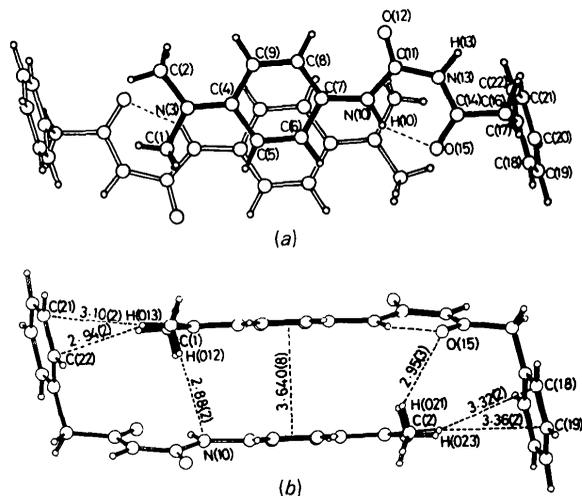
Table 2. *Bond lengths (Å) and bond angles (°)*

C(1)–N(3)	1·430 (3)	C(11)–N(13)	1·406 (2)
C(2)–N(3)	1·419 (3)	N(13)–C(14)	1·362 (2)
N(3)–C(4)	1·386 (2)	C(14)–O(15)	1·223 (2)
C(4)–C(5)	1·391 (2)	C(14)–C(16)	1·512 (2)
C(4)–C(9)	1·394 (2)	C(16)–C(17)	1·512 (2)
C(5)–C(6)	1·378 (2)	C(17)–C(18)	1·373 (2)
C(6)–C(7)	1·375 (2)	C(17)–C(22)	1·385 (2)
C(7)–C(8)	1·382 (2)	C(18)–C(19)	1·379 (3)
C(7)–N(10)	1·421 (2)	C(19)–C(20)	1·368 (3)
C(8)–C(9)	1·382 (2)	C(20)–C(21)	1·372 (3)
N(10)–C(11)	1·333 (2)	C(21)–C(22)	1·380 (3)
C(11)–O(12)	1·227 (2)		
C(1)–N(3)–C(2)	118·5 (2)	N(10)–C(11)–N(13)	115·7 (1)
C(1)–N(3)–C(4)	120·5 (2)	O(12)–C(11)–N(13)	118·6 (1)
C(2)–N(3)–C(4)	120·9 (2)	C(11)–N(13)–C(14)	128·8 (1)
N(3)–C(4)–C(5)	120·8 (2)	N(13)–C(14)–O(15)	123·2 (2)
N(3)–C(4)–C(9)	122·6 (2)	N(13)–C(14)–C(16)	115·2 (1)
C(5)–C(4)–C(9)	116·7 (2)	O(15)–C(14)–C(16)	121·7 (2)
C(4)–C(5)–C(6)	121·3 (2)	C(14)–C(16)–C(17)	109·6 (1)
C(5)–C(6)–C(7)	121·3 (2)	C(16)–C(17)–C(18)	120·7 (1)
C(6)–C(7)–C(8)	118·5 (1)	C(16)–C(17)–C(22)	120·5 (1)
C(6)–C(7)–N(10)	116·6 (1)	C(18)–C(17)–C(22)	118·7 (2)
C(8)–C(7)–N(10)	124·9 (1)	C(17)–C(18)–C(19)	121·0 (2)
C(7)–C(8)–C(9)	120·2 (2)	C(18)–C(19)–C(20)	120·2 (2)
C(4)–C(9)–C(8)	122·0 (2)	C(19)–C(20)–C(21)	119·3 (2)
C(7)–N(10)–C(11)	127·8 (1)	C(20)–C(21)–C(22)	120·9 (2)
N(10)–C(11)–O(12)	125·7 (1)	C(17)–C(22)–C(21)	119·9 (2)

Fig. 2. The overlapping mode of the two molecules around the inversion center (0,½,½): (*a*) projection along the normal to the mean plane of the benzene ring of the *p*-dimethylaminophenyl group and (*b*) side view. Several short intermolecular distances (Å) are shown.

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