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CI Pigment Yellow 65, α-(4-Methoxy-2-nitrophenylhydrazono)-α-aceto-2′-methoxyacetanilide

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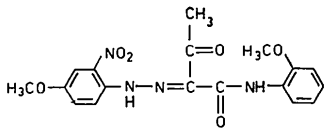
Abstract. 2-[(4-Methoxy-2-nitrophenyl)hydrazono]-*N*-(2-methoxyphenyl)-3-oxobutanamide, $C_{18}H_{18}N_4O_6$, $M_r = 386{\cdot}37$, monoclinic, $P2_1/c$, $a = 7{\cdot}2949\ (5)$, $b = 8{\cdot}9333\ (5)$, $c = 27{\cdot}5600\ (16)$ Å, $\beta = 94{\cdot}302\ (5)^\circ$, $V = 1791{\cdot}0\ (0{\cdot}2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}4330\ (2)$, $D_m = 1{\cdot}431\ (3)$ Mg m^{-3}, $F(000) = 808$, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 0{\cdot}83$ mm^{-1}, $R = 9{\cdot}5\%$ for 3047 independent non-zero intensities. The molecule exists as the hydrazone tautomer and four intramolecular hydrogen bonds keep it approximately planar. With the usual criterion there are two intermolecular hydrogen bonds per molecule but one is very weak.

Introduction. This article is one of a series (Whitaker, 1983*a*,*b*, 1984*a*,*b*, 1985*a*,*b*, 1986; Whitaker & Walker, 1985, 1987) concerned with the long-term aim of relating colour and crystal structure in acetoacetanilide pigments.

Previous structure determinations have indicated that the term 'azo-pigments', as applied to this group of pigments, is a misnomer; the azo bond is in fact a hydrazone bond (I). This conclusion has been confirmed by other investigators (Paulus, Rieper & Wagner, 1983; Brown & Yadav, 1984; Paulus, 1984). It had also been found that in pigments of this type the pigment molecule contains intramolecular hydrogen bonding and this generally tends to keep the molecule approximately planar. The one exception to this generalization (Paulus, Rieper & Wagner, 1983) contained methoxy side groups. The present pigment is an isomer of a previously determined one, CI Pigment Yellow 74 (Whitaker & Walker, 1987). The pigment is commercially available and is used in oil media, especially for latex paints for exterior use.



(I)

Experimental. Single crystals were obtained by the slow cooling of a hot saturated toluene solution (358 K) of the commercial pigment, Fanchon Yellow RN YH5790. Optical examination indicated that the crystals were monoclinic.

A crystal of size 0·60 × 0·22 × 0·15 mm was used for intensity measurements. These were collected on an Enraf–Nonius CAD-4 automatic four-circle diffractometer (Cu $K\alpha$ radiation). Least-squares analysis of 25 diffraction maxima with θ range 16·04–29·75° gave the cell constants. Space group $P2_1/c$ with b parallel to the blade face and perpendicular to the length, a parallel to the length of the crystal and c approximately perpendicular to the blade face. The observed density was measured by flotation.

The intensities were corrected for absorption [(North, Phillips & Mathews, 1968), linear absorption coefficient 0·83 mm^{-1}, maximum and minimum transmission factors 0·997 and 0·854 respectively] and

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Lorentz–polarization factor to give a total of 3292 intensities up to a maximum 2θ of 130·0°, all non-zero intensity with $-8 \leq h \leq 8$, $0 \leq k \leq 10$, $0 \leq l \leq 32$. These were merged to give 3047 independent reflections. The value of $R_{\rm int}$ was 2·5% for $0kl$ reflections.

The structure was solved using the direct methods of *MULTAN* (Germain, Main & Woolfson, 1970) after *SHELX*76 had failed. The refinement of the structure included a weighting function w such that $1/w = (\sigma^2 + 0{\cdot}03F^2)$; σ was obtained from the diffractometer counting statistics. After anisotropic refinement of the heavy atoms the H atoms were found from two successive difference Fourier syntheses; their positions confirmed the hydrazone tautomer. These were included with the isotropic temperature factors of the adjacent heavy atom at a distance of 1·05 Å. Refinement was then carried out until the shifts were less than one-tenth the appropriate standard deviation (Mason, 1964). No attempt was made to refine the parameters associated with the H atoms except for the methyl groups. Final $R = 0{\cdot}095$, $wR = 0{\cdot}096$. The final coordinates of the refined atoms, together with the isotropic temperature factors, are given in Table 1.* The comparatively high R value is attributed to the use of *all* data, which we consider to be methodologically more satisfactory than imposing an arbitrary cut-off (Hirshfeld & Rabinovich, 1973; Wilson, 1976, 1978). The maximum and minimum electron densities on the final difference Fourier synthesis were 0·48 and $-0{\cdot}74$ e Å^{-3} respectively.

Examination of the observed and calculated structure factors indicated that intense diffractions (*e.g.* 210, $\bar{2}11$, 011, 211, $\bar{2}21$ and 104) were affected by extinction. No correction was applied for this and these structure factors were included in the refinement.

During computing the following programs were used: *MULTAN* (Germain, Main & Woolfson, 1970) for direct methods (after *SHELX*76 had failed); Cambridge Crystallographic Package *SHELX*76 (Sheldrick, 1976) for data processing, Fourier synthesis and least-squares refinement; *BONDLA* for atomic distances and angles and *PARST* (Nardelli, 1982) for weighted least-squares planes. Figs. 1 and 2 were drawn by *PLUTO* (Motherwell & Clegg, 1978).

Table 1. *Parameters and standard deviations after anisotropic refinement*

$U_{\rm eq} = \exp[-8\pi^2 U(\sin^2\theta)/\lambda^2 \times 10^{-3}]$ (Cruickshank, 1956).

	x	y	z	$U_{\rm eq}$(Å^2)
C(1)	0·7839 (4)	0·0436 (3)	0·8507 (1)	34 (1)
N(4)	0·6981 (4)	−0·1041 (3)	0·8490 (1)	40 (1)
O(3)	0·6599 (5)	−0·1635 (3)	0·8873 (1)	62 (1)
O(4)	0·6593 (5)	−0·1630 (3)	0·8098 (1)	67 (1)
C(2)	0·8217 (4)	0·1023 (3)	0·8057 (1)	36 (1)
C(3)	0·8967 (4)	0·2433 (3)	0·8040 (1)	41 (1)
O(5)	0·9374 (3)	0·3136 (3)	0·7621 (1)	47 (1)
C(17)	0·8841 (6)	0·2413 (5)	0·7174 (1)	61 (1)
C(4)	0·9361 (4)	0·3228 (3)	0·8469 (1)	42 (1)
C(5)	0·8980 (4)	0·2628 (3)	0·8912 (1)	37 (1)
C(6)	0·8197 (4)	0·1208 (3)	0·8944 (1)	33 (1)
N(1)	0·7830 (3)	0·0624 (3)	0·9396 (1)	36 (1)
N(2)	0·8301 (3)	0·1411 (3)	0·9789 (1)	32 (1)
C(7)	0·7985 (4)	0·0917 (3)	1·0223 (1)	34 (1)
C(8)	0·8648 (2)	0·1947 (2)	1·0619 (1)	44 (1)
C(9)	0·9520 (6)	0·3402 (4)	1·0490 (1)	56 (1)
O(1)	0·8521 (4)	0·1627 (3)	1·1045 (1)	59 (1)
C(10)	0·7108 (4)	−0·0568 (3)	1·0305 (1)	35 (1)
O(2)	0·6642 (4)	−0·1388 (3)	0·9956 (1)	47 (1)
N(3)	0·6897 (3)	−0·0943 (3)	1·0771 (1)	40 (1)
C(11)	0·6242 (4)	−0·2308 (3)	1·0949 (1)	40 (1)
C(12)	0·6139 (4)	−0·2384 (3)	1·1454 (1)	38 (1)
O(6)	0·6603 (3)	−0·1088 (2)	1·1699 (1)	45 (1)
C(18)	0·6623 (5)	−0·1119 (4)	1·2215 (1)	51 (1)
C(13)	0·5586 (5)	−0·3696 (4)	1·1672 (1)	50 (1)
C(14)	0·5124 (5)	−0·4928 (4)	1·1386 (1)	56 (1)
C(15)	0·5177 (5)	−0·4864 (4)	1·0887 (1)	58 (1)
C(16)	0·5724 (4)	−0·3559 (4)	1·0665 (1)	49 (1)

Table 2. *Bond lengths* (Å) *and interatomic angles* (°)

O(3)—N(4)	1·231 (4)	C(7)—C(10)	1·497 (4)
O(4)—N(4)	1·217 (3)	C(10)—O(2)	1·235 (3)
N(4)—C(1)	1·459 (4)	C(10)—N(3)	1·348 (4)
C(1)—C(2)	1·393 (4)	N(3)—C(11)	1·411 (4)
C(2)—C(3)	1·375 (4)	C(11)—C(12)	1·400 (4)
C(3)—O(5)	1·367 (4)	C(12)—O(6)	1·370 (4)
O(5)—C(17)	1·422 (4)	O(6)—C(18)	1·421 (4)
C(3)—C(4)	1·390 (4)	C(12)—C(13)	1·390 (4)
C(4)—C(5)	1·381 (4)	C(13)—C(14)	1·380 (5)
C(5)—C(6)	1·397 (4)	C(14)—C(15)	1·382 (5)
C(6)—C(1)	1·396 (4)	C(15)—C(16)	1·388 (5)
C(6)—N(1)	1·395 (3)	C(16)—C(11)	1·400 (4)
N(1)—N(2)	1·314 (3)	N(1)—O(2)	2·562 (3)
N(2)—C(7)	1·314 (3)	N(1)—O(3)	2·601 (3)
C(7)—C(8)	1·480 (4)	N(3)—O(1)	2·666 (3)
C(8)—O(1)	1·219 (4)	N(3)—O(6)	2·586 (3)
C(8)—C(9)	1·502 (5)		

O(4)—N(4)—O(3)	121·5 (3)	C(10)—C(7)—N(2)	122·8 (2)
O(3)—N(4)—C(1)	119·2 (2)	C(7)—C(8)—C(9)	119·0 (2)
C(1)—N(4)—O(4)	119·3 (2)	C(9)—C(8)—O(1)	119·7 (3)
N(4)—C(1)—C(6)	121·7 (2)	O(1)—C(8)—C(7)	121·3 (3)
C(6)—C(1)—C(2)	123·1 (3)	C(7)—C(10)—N(3)	116·4 (2)
C(2)—C(1)—N(4)	115·2 (2)	N(3)—C(10)—O(2)	123·3 (3)
C(1)—C(2)—C(3)	118·7 (2)	O(2)—C(10)—C(7)	120·3 (2)
C(2)—C(3)—C(4)	119·8 (2)	C(10)—N(3)—C(11)	127·8 (2)
C(4)—C(3)—O(5)	116·1 (3)	N(3)—C(11)—C(12)	115·6 (2)
O(5)—C(3)—C(2)	124·1 (2)	C(12)—C(11)—C(16)	119·0 (3)
C(3)—O(5)—C(17)	117·5 (3)	C(16)—C(11)—N(3)	125·4 (3)
C(3)—C(4)—C(5)	120·7 (3)	C(11)—C(12)—O(6)	114·8 (2)
C(4)—C(5)—C(6)	121·2 (2)	O(6)—C(12)—C(13)	124·7 (3)
C(5)—C(6)—N(1)	120·2 (2)	C(13)—C(12)—C(11)	120·6 (3)
N(1)—C(6)—C(1)	123·4 (2)	C(12)—O(6)—C(18)	117·4 (3)
C(1)—C(6)—C(5)	116·4 (2)	C(12)—C(13)—C(14)	119·5 (3)
C(6)—N(1)—N(2)	118·7 (2)	C(13)—C(14)—C(15)	120·7 (3)
N(1)—N(2)—C(7)	121·2 (2)	C(14)—C(15)—C(16)	120·2 (3)
N(2)—C(7)—C(8)	113·1 (2)	C(15)—C(16)—C(11)	119·9 (3)
C(8)—C(7)—C(10)	124·1 (2)		

Discussion. Bond lengths and angles are given in Table 2. Comparison of the observed bond lengths with accepted bond lengths (*International Tables for X-ray Crystallography,* 1968) confirms that the hydrazone tautomer is the better model, thus agreeing with the

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* Lists of structure factors, anisotropic thermal parameters, calculated H-atom parameters and heavy-atom peak heights have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44201 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

previous determinations. Fig. 1 gives the proposed molecular structure projected on to the plane containing the atoms C(2), C(3) and C(13).

In addition the interatomic distances N(1)—O(2), N(1)—O(3), N(3)—O(1) and N(3)—O(6) suggest that there is a bifurcated hydrogen bond from N(1) to O(2) and O(3) and another from N(3) to O(1) and O(6). The first of these has been found in previously determined structures with similar values of the bond lengths. The second occurs in CI Pigment Yellow 74 (Whitaker & Walker, 1987), again with similar bond lengths. These hydrogen bonds will inhibit rotation about neighbouring bonds and tend to hold parts of the molecule planar.

There would appear to be no abnormal bond lengths. In fact, if one considers the mean values from this structure and its isomer, CI Pigment Yellow 74 (Whitaker & Walker, 1987), no individual bond lengths in either structure (excluding intramolecular hydrogen bonds) differ by more than three times the standard deviation from the mean. This makes the dimethoxy compound of Paulus, Rieper & Wagner (1983) more obviously unusual. It has already been pointed out that the three nominally single carbon–carbon bonds [here named C(7)—C(8), C(8)—C(9) and C(7)—C(10)] in this dimethoxy structure are significantly different from each other, 1·462 (3), 1·501 (3) and 1·477 (3) Å respectively. In CI Pigment Yellow 74 (Whitaker & Walker, 1987) they are 1·492 (3), 1·494 (4) and 1·488 (3) Å while in the present structure they are 1·480 (4), 1·502 (5) and 1·497 (4) Å, both sets being essentially equal. This significant distortion in the dimethoxy structure of Paulus, Rieper & Wagner (1983) may be the reason why their molecule is substantially non-planar.

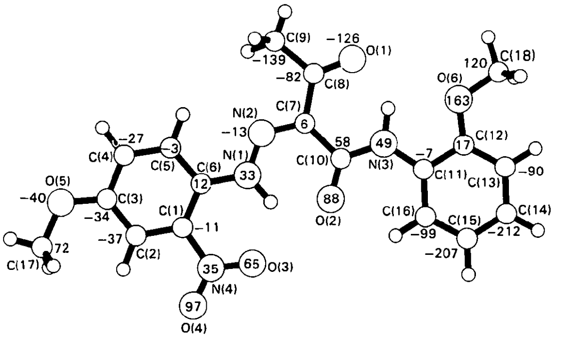

Fig. 1. Structure of the molecule projected on to the plane containing C(2), C(3) and C(13). The deviations of the atoms (in 10^{-3} Å) from the weighted least-squares plane of the molecule are also given. The e.s.d.'s in the atomic coordinates correspond to a mean of 0·003 Å.

Although the present molecule is almost planar, nearly all atoms show significant deviations from this plane; these deviations are given in Fig. 1. A more detailed examination shows that the benzene rings are inclined at an angle of 5·30 (9)° with respect to each other; this compares with 5·68 (7)° in the case of CI Pigment Yellow 74 (Whitaker & Walker, 1987) and 37·65 (8)° for the other dimethoxy compound studied (Paulus, Rieper & Wagner, 1983).

The *a*-axis projection of the structure (Fig. 2) shows that the molecules lie in columns parallel to this axis; adjacent molecules within the columns lie antiparallel. The normal to the weighted molecular plane is 24·04 (2)° offset with respect to the column axis; this plane makes an angle of 1·55 (1)° with the ($\bar{2}10$) plane. All intermolecular distances (excluding those involving hydrogen) below 3·50 Å were calculated (these have been deposited). The two short distances C(18)—O(4) = 3·158 and C(17)—O(1) = 3·217 Å can be compared with the values for the van der Waals distance for methyl–oxygen of 3·40 (Pauling, 1960) and 3·28 Å [Bondi (1964), obtained by combining the methyl–methyl contact distance, 3·57 Å, with his van der Waals radius for oxygen, 1·50 Å]. This suggests the presence of intermolecular hydrogen bonds.

Sutor (1963) undertook an investigation of short intermolecular and intramolecular C···O contacts, mainly in the region of 3·1 Å. Although, in many of the compounds considered, the positions of the H atom had not been directly determined, many of these short distances could be due to C—H···O. It was found that in the case of methylidene (CH) groups, the C—H···O configuration was approximately linear and the H···O distances less than 2·6 Å [the sum of the van der Waals radii according to Pauling (1960); Bondi (1964) gives

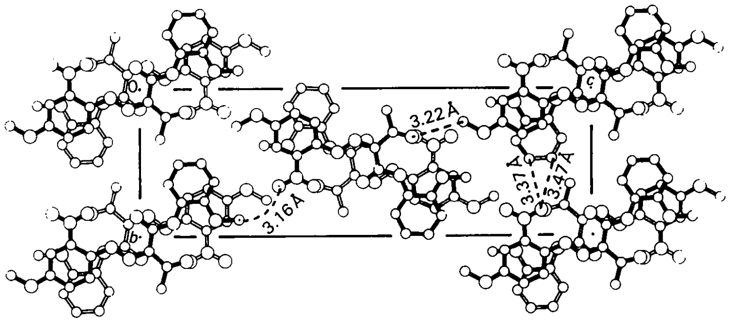

Fig. 2. The packing of CI Pigment Yellow 65 molecules in the unit cell, *a*-axis projection. Intercolumnar intermolecular distances less than 3·50 Å shown. The molecules at the higher level in the cell (*i.e.* those with larger *x* coordinates) are indicated by solid bonds.

Table 3. *Intermolecular distances* (Å) *and angles* (°) *about the methyl groups* C(17)H$_3$ *and* C(18)H$_3$

	x	*y*	*z*				
C(18)	0·6623 (5)	−0·1119 (4)	1·2215 (1)	C(18)—O(4)	3·158 (4)	C(18)—H(181)—O(4)	121 (3)
H(181)	0·7374 (46)	−0·1874 (41)	1·2339 (13)	C(18)—H(181)	0·918 (35)	C(18)—H(182)—O(4)	92 (2)
H(182)	0·5264 (48)	−0·1213 (37)	1·2352 (12)	C(18)—H(182)	1·090 (36)	C(18)—H(183)—O(4)	83 (2)
H(183)	0·7350 (45)	−0·0145 (41)	1·2351 (12)	C(18)—H(183)	1·072 (35)		
O(4)	0·6593 (5)	−0·3370 (3)	1·3098 (1)	H(181)—O(4)	2·583 (36)		
				H(182)—O(4)	2·929 (33)		
				H(183)—O(4)	3·433 (33)		
C(17)	0·8841 (6)	0·2413 (5)	0·7174 (1)	C(17)—O(1)	3·217 (4)	C(17)—H(171)—O(1)	72 (2)
H(171)	0·7628 (57)	0·2060 (45)	0·7134 (13)	C(17)—H(171)	0·938 (41)	C(17)—H(172)—O(1)	130 (2)
H(172)	0·9174 (51)	0·3191 (43)	0·6950 (14)	C(17)—H(172)	0·971 (39)	C(17)—H(173)—O(1)	not calc.
H(173)	0·9671 (51)	0·1380 (44)	0·7131 (13)	C(17)—H(173)	1·115 (39)		
O(1)	0·8521 (4)	0·3373 (3)	0·6045 (1)	H(171)—O(1)	3·330 (38)		
				H(172)—O(1)	2·510 (39)		
				H(173)—O(1)	>3·5		

2·70 Å], but for methylene (CH$_2$) and methyl (CH$_3$) groups this was not necessary, and in the cases considered the angle C—H···O varied from 102 to 147° and the distance H···C could be larger than 2·6 Å. It was suggested that this could be due to steric hindrance from other atoms of the methylene or methyl groups.

Examination of the distances about the methyl groups (Table 3) suggests that there is a hydrogen bond C(18)—H(181)···O(4), and there also appears to be a weak hydrogen bond, C(17)—H(172)···O(1). However, the latter bond is only slightly shorter than the van der Waals distance given by Bondi (1964) (3·28 Å) and so must be very weak indeed. The first of these tends to cause the molecules to lie in puckered chains parallel to **c**.

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4,4′-Bipyridinium(2+) Dinitrate

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Abstract. $C_{10}H_{10}N_4O_6$, $M_r = 282·2$, monoclinic, $C2/c$, $a = 16·08$ (3), $b = 3·785$ (6), $c = 18·85$ (3) Å, $\beta = 98·16$ (2)°, $U = 1135·6$ Å^3, $Z = 4$, $D_x = 1·65$, $D_m = 1·64$ (1) Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0·76$ mm^{-1}, $F(000) = 584$, $T = 291$ (1) K, $R = 0·048$ for 610 unique reflections. The planar centrosymmetric

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