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## 4-(2,3-Dichlorobenzylideneamino)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one

The title Schiff base compound,  $C_{18}H_{15}Cl_2N_3O$ , was synthesized by the reaction of 4-amino-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one and 2,3-dichlorobenzaldehyde in MeOH solution. There are two molecules in the asymmetric unit. As expected, the compound adopts a *trans* configuration about the central C=N bond. In the crystal structure, molecules are linked through weak C—H...O hydrogen-bonding interactions.

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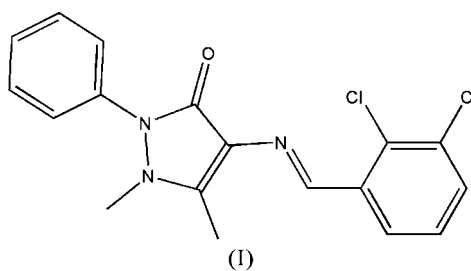
## Key indicators

Single-crystal X-ray study  
 $T = 295\text{ K}$   
 Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.057  
 $wR$  factor = 0.134  
 Data-to-parameter ratio = 16.3

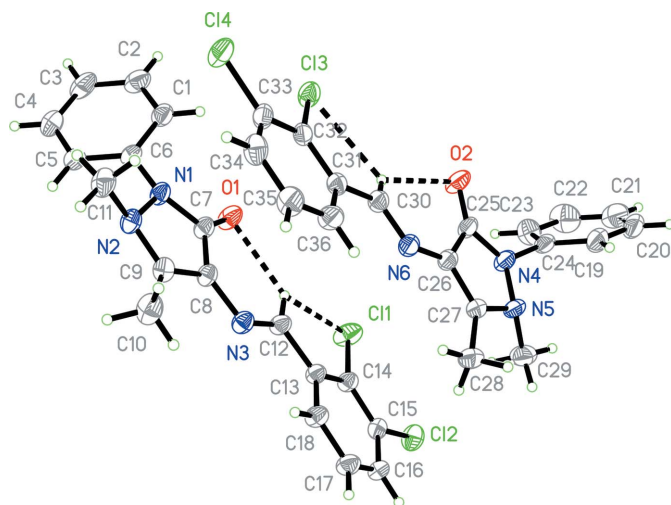
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Comment

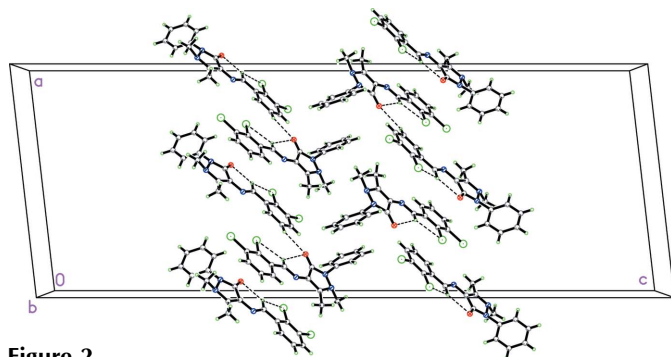
Antipyrine and its derivatives exhibit a wide range of biological activities and applications (Yadav *et al.*, 2003; Ismail, 2000; Abd El Rehim *et al.*, 2001). A few crystal structures of antipyrine derivatives have been investigated (Liang *et al.*, 2002; Li & Zhang, 2004, 2005; Zhang & Li, 2005; You, *et al.*, 2004, 2006; Wen, 2005). Schiff bases of salicylaldehyde have demonstrated significant biological activity and new examples are being tested for their antitumor, antimicrobial and antiviral activity (Tarafder *et al.*, 2002; Cukurovali *et al.*, 2002; Ali *et al.*, 2002). As an extension of our work (Sun *et al.*, 2006) on the structural characterization of antipyrine derivatives, the title compound, (I), is reported here.



The asymmetric unit of (I) consists of two independent molecules (Fig. 1). In both of these, the bond lengths and angles are in normal ranges, close to those observed in similar antipyrine Schiff bases cited above. The dihedral angle between the N1/N2/C7–C9 pyrazoline ring and the C1–C6 benzene ring is  $47.8(3)^\circ$  and that between the N4/N5/C25–C27 pyrazoline ring and the C19–C24 benzene ring is  $61.7(3)^\circ$ . Atom O1 deviates from the pyrazoline mean plane by  $0.132(3)\text{ \AA}$ , whereas atoms C10 and C11 deviate from it, on the opposite side, by  $0.133(3)$  and  $0.681(4)\text{ \AA}$ , respectively. Atom O2 deviates from the other pyrazoline mean plane by  $0.153(3)\text{ \AA}$ , whereas atoms C28 and C29 deviate from it, on the opposite side, by  $0.059(2)$  and  $0.771(4)\text{ \AA}$ , respectively. As a result of conjugation through the imino double bonds, the pyrazoline and C13–C18 and C31–C36 benzene ring systems in both molecules are nearly coplanar, the dihedral angle



**Figure 1**  
The asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are shown as dashed lines.



**Figure 2**  
Part of the crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

between the N1/N2/C7–C9 pyrazoline ring and the C13–C18 benzene ring being  $11.5(5)^\circ$  [mean deviation from the combined mean plane is  $0.087(5) \text{ \AA}$ ] and that between the N4/N5/C25–C27 pyrazoline ring and the C31–C36 benzene ring is  $11.7(5)^\circ$  [mean deviation from the combined plane is  $0.004(5) \text{ \AA}$ ]. As expected, the two molecular structures adopt the same *trans* configurations about the C12=N3 and C30=N6 bonds as the other antipyrine derivatives that have been reported.

In the crystal structure, C17–H17 $\cdots$ O2<sup>i</sup> and C35–H35 $\cdots$ O1<sup>ii</sup> non-classical weak hydrogen bonds link the molecules into one-dimensional chains along the *b* axis (Fig. 2 and Table 1). In addition, the *ortho* Cl atoms participate in the formation of intramolecular weak hydrogen bonds (Table 1).

## Experimental

All the chemicals were obtained from commercial sources and used without purification. 4-Amino-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (2 mmol, 0.406 g) and an equimolar quantity of 2,3-dichlorobenzaldehyde (2 mmol, 0.350 g) were dissolved in methanol (15 ml). The mixture was stirred for 30 min at room temperature to give a clear yellow solution. The resulting solution was kept in air for

12 d, and yellow prism-shaped crystals of (I) were formed at the bottom of the vessel on slow evaporation of the methanol (yield 89.7%). Analysis calculated for C<sub>18</sub>H<sub>15</sub>Cl<sub>2</sub>N<sub>3</sub>O: C 60.01, H 4.20, N 11.66%; found: C 59.89, H 4.17, N 11.59%.

## Crystal data

C<sub>18</sub>H<sub>15</sub>Cl<sub>2</sub>N<sub>3</sub>O  
*M<sub>r</sub>* = 360.23  
 Monoclinic, *C2/c*  
*a* = 18.9602 (8) Å  
*b* = 7.1044 (3) Å  
*c* = 51.387 (2) Å  
 $\beta$  =  $96.529(1)^\circ$   
*V* = 6877.0 (5) Å<sup>3</sup>

*Z* = 16  
*D<sub>x</sub>* = 1.392 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.39 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Prism, yellow  
 0.35 × 0.08 × 0.07 mm

## Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.956, *T<sub>max</sub>* = 0.973

35938 measured reflections  
 7114 independent reflections  
 5532 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.042  
 $\theta_{\text{max}}$  =  $26.5^\circ$

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.057  
*wR* (*F*<sup>2</sup>) = 0.134  
*S* = 1.09  
 7114 reflections  
 437 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 7.688P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.37 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H $\cdots$ <i>A</i>	<i>D</i> –H	H $\cdots$ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> –H⋯ <i>A</i>
C17–H17 $\cdots$ O2 <sup>i</sup>	0.93	2.52	3.153 (4)	125
C12–H12 $\cdots$ Cl1	0.93	2.70	3.067 (3)	104
C12–H12 $\cdots$ O1	0.93	2.35	3.025 (3)	129
C35–H35 $\cdots$ O1 <sup>ii</sup>	0.93	2.65	3.221 (3)	121
C30–H30 $\cdots$ Cl3	0.93	2.68	3.059 (3)	105
C30–H30 $\cdots$ O2	0.93	2.42	3.061 (3)	126

Symmetry codes: (i)  $x + \frac{1}{2}, y + \frac{1}{2}, z$ ; (ii)  $x, y + 1, z$ .

All H atoms were positioned geometrically (C–H = 0.93 or 0.96 Å) and constrained to ride on their parent atoms with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for aromatic H atoms or *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C) for methyl H atoms.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT-Plus (Bruker, 2002); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2002); software used to prepare material for publication: SHELXL97.

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