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# 2,3,4,6-Tetraphenyl-2*H*-pyrazolo[3,4-*d*]-pyridazin-7(6*H*)-one

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The title compound, $C_{29}H_{20}N_4O$, is a derivative of 2*H*-pyrazolo[3,4-*d*]pyridazine and is non-planar, although consisting of planar fragments. The structure consists of planar fragments. There are two independent molecules in the asymmetric unit. The dihedral angle between the fused pyridazine and pyrazole rings is 2.61 (11)° in molecule *A* [3.19 (11)° in molecule *B*]. The crystal structure is stabilized by intramolecular and intermolecular C—H···O interactions.

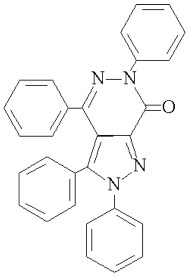
**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean $\sigma$(C–C) = 0.004 Å
*R* factor = 0.050
*wR* factor = 0.089
Data-to-parameter ratio = 12.8

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

## Comment

Pyrazole derivatives have been the subject of much research because of their importance in various applications and their widespread potential biological and pharmacological activities, such as antimicrobial (Mahajan *et al.*, 1991), antiviral (Baraldi *et al.*, 1998), antitumor (Hatheway *et al.*, 1978; Katayama & Oshiyama, 1997), antifungal (Chen & Li, 1998), pesticidal (Londershausen, 1996), anticonvulsant (Lepage & Hublot, 1992), antihistaminic (Mishra *et al.*, 1998) and antidepressant activities (Bailley *et al.*, 1985), as well as their interesting properties as commercially important dyestuffs (Neunhoeffer *et al.*, 1959; Baroni & Kovyrzina, 1961). The reaction of 4-benzoyl-5-phenyl-2,3-dihydro-2,3-furandione with various phenylhydrazones and phenylhydrazine leads to pyrazole carboxylic acid and pyridazinones (Akçamur *et al.*, 1986; Akçamur *et al.*, 1997; Şener et al., 2002; Dinçer *et al.*, 2004). 4-Aroyl-5-aryl-2,3-dihydro-2,3-furandiones represent easily accessible building blocks for the synthesis of heterocyclic systems (Saalfrank *et al.*, 1991; Terpetschnig *et al.*, 1991; Yıldırım & İlhan, 1997; Hökelek *et al.*, 2002; Yıldırım & Kandemirli, 2004). In view of these important properties, we have undertaken the X-ray diffraction study of the title compound, (I).



(I)

Fig. 1 shows the molecular structure and conformation of (I), with the atomic numbering scheme. As seen in Fig. 1, there are two crystallographically independent molecules, *A* and *B*, in the asymmetric unit of (I), with bond lengths and angles

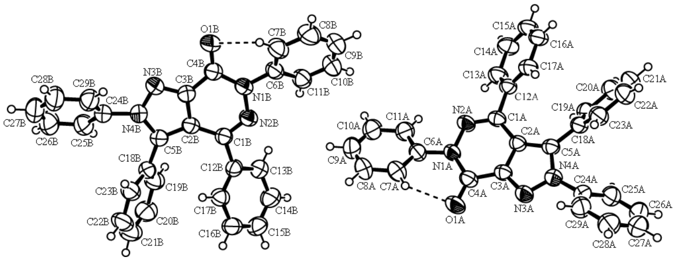


**Figure 1**

The two independent molecules of (I), with 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms are shown as small spheres of arbitrary radii and dashed lines denote the intramolecular C—H···O interactions.

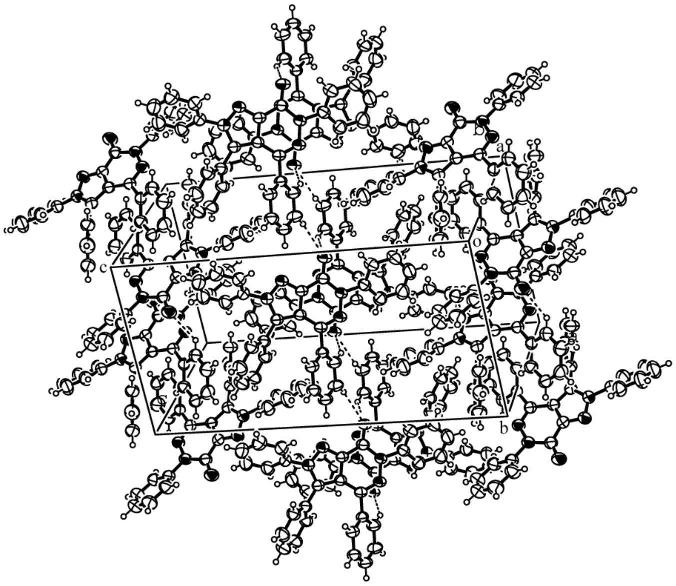


**Figure 2**

An *ORTEP*-3 (Farrugia, 1997) drawing of (I), showing the molecular packing and the intermolecular interactions as dashed lines.

that agree with each other. Selected bond lengths and angles are listed in Table 1.

The title compound, (I), contains one pyridazine ring (ring *A*; N1/N2/C1–C4), which is fused with the pyrazole ring (ring *B*; N3/N4/C2/C3/C5), four phenyl rings and an O atom (O1) attached to the pyridazine ring at C4. Although both the pyridazine and the pyrazole rings are planar, they are not coplanar; the dihedral angle between the pyridazine and pyrazole rings is 2.61 (11)° in molecule *A* [3.19 (11)° in molecule *B*].

The phenyl ring substituents attached to the pyrazole ring moiety at C5 and N4 are twisted by 55.01 (12) and 50.98 (13)°, respectively, with respect to the mean plane of the pyrazole ring in molecule A [61.02 (12) and 43.40 (13)° in molecule B].

The pyridazine ring forms dihedral angles of 25.59 (12) and 47.79 (10)° with the phenyl rings substituted at N1 and C1 in molecule *A* [30.51 (12) and 42.49 (11)° in molecule *B*], respectively.

In the title structure, an intramolecular C—H···O interaction forms a six-membered O1/C4/N1/C6/C7/H7 closed ring, which is not planar and which is fused with both the pyridazine ring and the C6–C11 ring. Three intermolecular interactions are observed in the structure. Atoms H14*A* and H13*A* of the phenyl ring (C14*A* and C13*A*) interact with the O atom (O1*A*) substituted at C4*A* [C14*A*···O1*A*$^{i}$ = 3.255 (3) Å and C13*A*···O1*A*$^{ii}$ = 3.255 (3) Å; symmetry codes: (i) $x$, $y + 1$, $z$; (ii) $1 - x$, $1 - y$, $1 - z$]. In addition, atom H13*B* of the phenyl ring (C13*B*) interacts with the O atom (O1*B*) substituted at C4*B* [C13*B*···O1*B*$^{iii}$ = 3.257 (3) Å; symmetry code: (iii) $1 - x$, $1 - y$, $-z$]. The O atom acts as a single acceptor for all intermolecular interactions. The crystal structure is stabilized by these intramolecular and intermolecular interactions.

## Experimental

4-Benzoyl-1,5-diphenyl-1*H*-pyrazole-3-carboxylic acid (0.49 g, 1.30 mmol) or, alternatively, 4-benzoyl-1,5-diphenyl-1*H*-pyrazole-3-carboxylic acid chloride (0.50 g, 1.30 mmol), obtained easily from 4-benzoyl-5-phenyl-2,3-dihydro-2,3-furandione and phenylhydrazine (Akçamur *et al.*, 1997), and phenylhydrazine (0.15 g, 1.34 mmol) were reacted in boiling xylene for 3 h. The solvent was removed by evaporation and the oily residue was triturated with dry ether to give a crude solid, which was then recrystallized from ethanol, yielding pure (I) (0.41 g, 70%); m.p. 489–491 K. Solvents were dried by refluxing with the appropriate drying agents and distilled before use. All other reagents were purchased from Merck, Fluka, Aldrich and Acros Chemical Co., and used without further purification. Analysis calculated for $C_{29}H_{20}N_4O$: C 79.07, H 4.58, N 12.72%; found: C 79.14, H 4.69, N 12.69%.

*Crystal data*

$C_{29}H_{20}N_4O$
$M_r = 440.49$
Triclinic, $P\bar{1}$
$a = 10.2616\ (12)$ Å
$b = 10.5057\ (12)$ Å
$c = 21.264\ (2)$ Å
$\alpha = 95.064\ (9)^\circ$
$\beta = 93.438\ (9)^\circ$
$\gamma = 102.158\ (9)^\circ$
$V = 2225.0\ (4)$ Å$^3$

$Z = 4$
$D_x = 1.315$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 15 351 reflections
$\theta = 1.9$–$26.9^\circ$
$\mu = 0.08$ mm$^{-1}$
$T = 293\ (2)$ K
Prism, colorless
0.50 × 0.33 × 0.23 mm

*Data collection*

Stoe IPDS II diffractometer
$\omega$ scans
28 743 measured reflections
7844 independent reflections
3864 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.138$
$\theta_{\rm max} = 25.0^\circ$
$h = -12 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -25 \rightarrow 25$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.089$
$S = 0.81$
7844 reflections
614 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0101P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -0.24$ e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0137 (8)

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**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1*A*—C4*A* | 1.220 (2) | O1*B*—C4*B* | 1.208 (2) |
| N1*A*—C4*A* | 1.385 (3) | N1*B*—N2*B* | 1.390 (2) |
| N1*A*—N2*A* | 1.389 (2) | N1*B*—C4*B* | 1.397 (3) |
| N1*A*—C6*A* | 1.444 (3) | N1*B*—C6*B* | 1.445 (3) |
| N2*A*—C1*A* | 1.299 (3) | N2*B*—C1*B* | 1.301 (3) |
| N3*A*—C3*A* | 1.330 (2) | N3*B*—C3*B* | 1.330 (3) |
| N3*A*—N4*A* | 1.357 (2) | N3*B*—N4*B* | 1.362 (2) |
| N4*A*—C5*A* | 1.372 (3) | N4*B*—C5*B* | 1.369 (2) |
| N4*A*—C24*A* | 1.432 (3) | N4*B*—C24*B* | 1.448 (3) |
| C1*A*—C2*A* | 1.437 (3) | C1*B*—C2*B* | 1.442 (3) |
| C1*A*—C12*A* | 1.485 (3) | C1*B*—C12*B* | 1.475 (2) |
| C2*A*—C5*A* | 1.386 (3) | C2*B*—C5*B* | 1.395 (3) |
| C2*A*—C3*A* | 1.394 (3) | C2*B*—C3*B* | 1.403 (3) |
| C3*A*—C4*A* | 1.444 (3) | C3*B*—C4*B* | 1.450 (3) |
| C5*A*—C18*A* | 1.471 (3) | C5*B*—C18*B* | 1.471 (3) |
| | | | |
| C4*A*—N1*A*—C6*A* | 122.71 (19) | N2*B*—N1*B*—C6*B* | 112.21 (16) |
| N2*A*—N1*A*—C6*A* | 111.82 (17) | C4*B*—N1*B*—C6*B* | 122.08 (17) |
| C1*A*—N2*A*—N1*A* | 120.41 (17) | C1*B*—N2*B*—N1*B* | 121.21 (17) |
| N3*A*—N4*A*—C5*A* | 113.76 (17) | N3*B*—N4*B*—C5*B* | 114.18 (17) |
| N3*A*—N4*A*—C24*A* | 117.73 (18) | N3*B*—N4*B*—C24*B* | 116.38 (16) |
| C5*A*—N4*A*—C24*A* | 128.47 (19) | C5*B*—N4*B*—C24*B* | 129.42 (19) |
| N2*A*—C1*A*—C12*A* | 114.33 (19) | N2*B*—C1*B*—C12*B* | 112.60 (18) |
| C2*A*—C1*A*—C12*A* | 124.6 (2) | C2*B*—C1*B*—C12*B* | 127.1 (2) |
| O1*A*—C4*A*—N1*A* | 122.9 (2) | O1*B*—C4*B*—N1*B* | 123.1 (2) |
| O1*A*—C4*A*—C3*A* | 124.8 (2) | O1*B*—C4*B*—C3*B* | 125.6 (2) |
| N4*A*—C5*A*—C18*A* | 122.10 (19) | N4*B*—C5*B*—C18*B* | 123.30 (19) |
| C2*A*—C5*A*—C18*A* | 133.11 (19) | C2*B*—C5*B*—C18*B* | 131.64 (18) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7*A*—H7*A*···O1*A* | 0.93 | 2.23 | 2.770 (3) | 116 |
| C7*B*—H7*B*···O1*B* | 0.93 | 2.32 | 2.814 (3) | 113 |
| C14*A*—H14*A*···O1*A*$^{i}$ | 0.93 | 2.44 | 3.255 (3) | 147 |
| C13*A*—H13*A*···O1*A*$^{ii}$ | 0.93 | 2.46 | 3.255 (3) | 144 |
| C13*B*—H13*B*···O1*B*$^{iii}$ | 0.93 | 2.52 | 3.257 (3) | 136 |

Symmetry codes: (i) $x, 1+y, z$; (ii) $1-x, 1-y, 1-z$; (iii) $1-x, 1-y, -z$.

H atoms were positioned geometrically and treated using a riding model, fixing the C—H distances at 0.93 Å for the phenyl rings. The displacement parameters of the H atoms were constrained as $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom). The high $R_{\rm int}$ value indicates that the overall quality of the data may be poor due to the crystal quality. No further options were available to increase the intensity data.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *PLATON* (Spek, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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