

2-(2-Methylphenyl)-4,5-diphenyl-1*H*-imidazole

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Key indicators

Single-crystal X-ray study
 $T = 120$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.041
 wR factor = 0.103
 Data-to-parameter ratio = 8.7

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

In the title molecule, $\text{C}_{22}\text{H}_{18}\text{N}_2$, all bond lengths and angles are normal. Intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds with an $\text{N}\cdots\text{N}$ distance of 2.933 (2) Å, link the molecules into chains running along the c axis. The crystal packing is further stabilized by van der Waals forces.

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Comment

Several heterocyclic compounds with aryl substituents have previously been reported to exhibit anti-inflammatory activity in animals (Almirante *et al.*, 1965; Marchetti *et al.*, 1968). Of the various polyaryl heterocycles, certain 4,5-diphenyl-2-substituted imidazoles exhibited anti-inflammatory activity comparable to phenylbutazone in the carrageenan rat paw edema test (Lombardino & Wiseman, 1974). In view of this importance, we report here the crystal structure of the title compound, (I), which is a 4,5-diphenyl-2-substituted imidazole derivative.

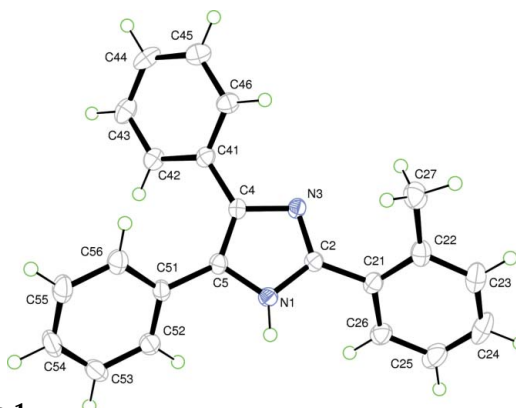
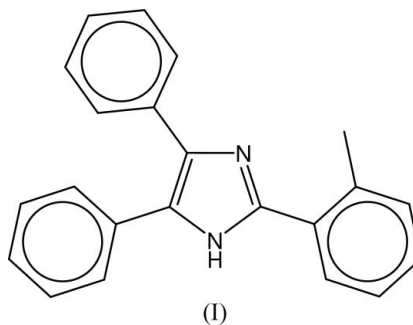


Figure 1
View of (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. H atoms are represented by circles of arbitrary radii.

The bond lengths and angles in (I) (Fig. 1) are in good agreement with the literature values (Allen *et al.*, 1987). The imidazole ring makes dihedral angles of 41.2 (1), 31.5 (1) and 41.7 (1)° with the C21–C26, C41–C46 and C51–C56 aromatic rings, respectively. In the solid state, intermolecular N–H···N hydrogen bonds (Table 1) link the molecules into *C*(4) chains (Bernstein *et al.*, 1995) running along the *c* axis. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Experimental

A mixture of benzil (5.25 g, 0.025 mol), ammonium acetate (10 g, 0.129 mol) and 2-methylbenzaldehyde (0.018 mol) in glacial acetic acid (50 ml) was heated under reflux for 1–2 h. The product was recrystallized from aqueous ethanol (yield 80%, m.p. 484–486 K).

Crystal data

$C_{22}H_{18}N_2$	$Z = 4$
$M_r = 310.38$	$D_x = 1.220 \text{ Mg m}^{-3}$
Monoclinic, <i>Cc</i>	Mo $K\alpha$ radiation
$a = 10.7538 (5) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$b = 19.3999 (9) \text{ \AA}$	$T = 120 (2) \text{ K}$
$c = 8.7900 (3) \text{ \AA}$	Rod, colourless
$\beta = 112.886 (2)^\circ$	$0.36 \times 0.06 \times 0.04 \text{ mm}$
$V = 1689.44 (13) \text{ \AA}^3$	

Data collection

Nonius KappaCCD area-detector diffractometer	10671 measured reflections
φ and ω scans	1945 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	1744 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.745$, $T_{\max} = 0.927$ (expected range = 0.801–0.997)	$R_{\text{int}} = 0.059$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.7664P]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
1945 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
223 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0089 (16)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1···N3 ⁱ	0.88 (3)	2.07 (3)	2.933 (3)	168 (3)

Symmetry code: (i) $x, -y, z - \frac{1}{2}$.

The position of the amine H atom was determined from a difference Fourier map and refined freely along with its isotropic displacement parameter. The methyl H atoms were constrained to an ideal geometry (C–H = 0.98 Å), with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, but were allowed to rotate freely about the C–C bond. The remaining H atoms were placed in geometrically idealized positions (C–H = 0.95 Å) and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) =$

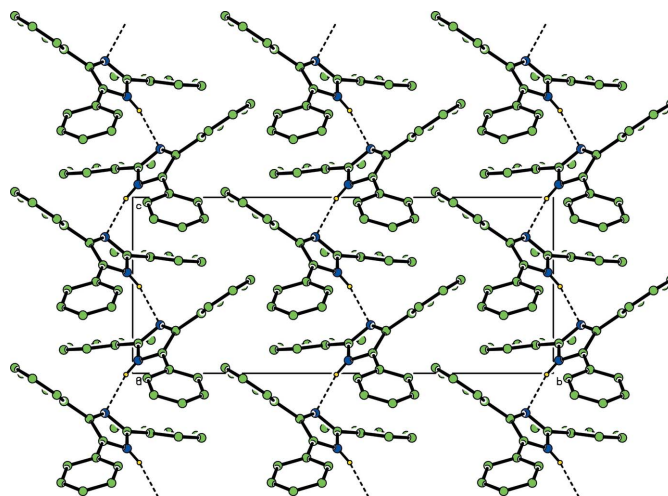


Figure 2

The crystal packing of (I), viewed along the *a* axis. The intermolecular N–H···N hydrogen bonds are shown as dashed lines. All the H atoms, except those involved in hydrogen bonding, have been omitted for clarity.

$1.2U_{\text{eq}}(\text{C})$. Owing to the absence of any significant anomalous scatterers in the molecule, the 1433 Friedel pairs were merged before the final refinement.

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1994); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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