

T. Seethalakshmi,^a A. Puratchikody,^b Daniel E. Lynch,^c P. Kaliannan^a and S. Thamotharan^{d*}

^aSchool of Physics, Bharathidasan University, Tiruchirappalli 620 024, India, ^bDepartment of Pharmacy, Bharathidasan University of Technology, Bharathidasan University, Tiruchirappalli 620 024, India, ^cFaculty of Health and Life Sciences, Coventry University, Coventry CV1 5FB, England, and ^dMolecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India

Correspondence e-mail: thamu_as@yahoo.com

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>.

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

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.

Received 26 May 2006

Accepted 2 June 2006

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.

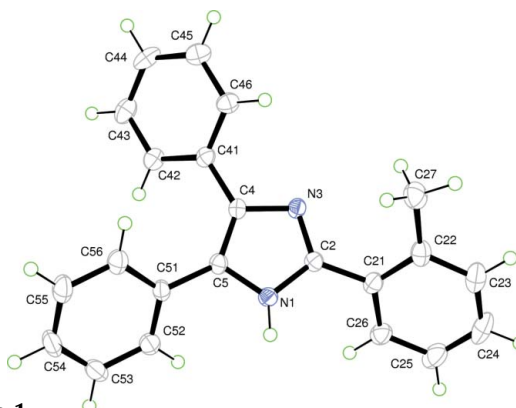
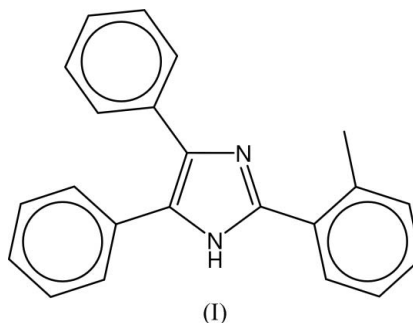


Figure 1
 View of (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. H atoms are represented by circles of arbitrary radii.

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 (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots N3^i$	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 ($C-H = 0.98 \text{ \AA}$), with $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$, but were allowed to rotate freely about the $C-C$ bond. The remaining H atoms were placed in geometrically idealized positions ($C-H = 0.95 \text{ \AA}$) and constrained to ride on their parent atoms with $U_{\text{iso}}(H) =$

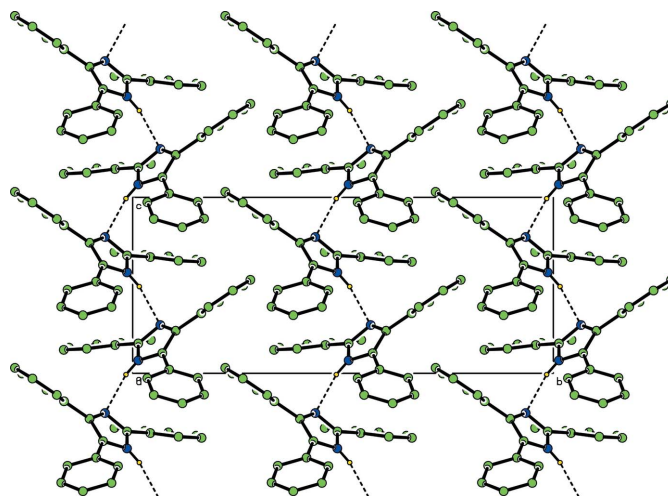


Figure 2

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.

$1.2U_{\text{eq}}(C)$. 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.

The authors thank the EPSRC National Crystallography Service (Southampton, England). TS thanks Professors V. Parthasarathi, School of Physics and M. Nallu, School of Chemistry, Bharathidasan University, Tiruchirappalli, for their generous help.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Almirante, L., Polo, L., Mugnaini, A., Provinciali, E., Rugarli, P., Biancotti, A., Gamba, A. & Murmann, W. (1965). *J. Med. Chem.* **8**, 305–312.
- Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Hooft, R. W. W. (1998). COLLECT. Nonius BV, Delft, The Netherlands.
- Lombardino, J. G. & Wiseman, E. H. (1974). *J. Med. Chem.* **17**, 1182–1188.
- Marchetti, E., Mattalia, G. & Rosnati, V. (1968). *J. Med. Chem.* **11**, 1092–1093.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.
- Sheldrick, G. M. (2003). SADABS. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.