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Key indicators

Single-crystal X-ray study
T = 393 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.047
wR factor = 0.119
Data-to-parameter ratio = 15.3

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

2-[4-(Dimethylamino)phenyl]-4,5-diphenyl-1H-imidazole isopropanol solvate

The title compound, $\text{C}_{23}\text{H}_{21}\text{N}_3 \cdot \text{C}_3\text{H}_8\text{O}$, crystallizes with two independent molecules and two solvent molecules in the asymmetric unit. These are connected through hydrogen bonds between the NH group of the imidazole ring and the O atom of the isopropanol solvent molecule, as well as between the N atom of the imidazole ring and the OH group of the isopropanol solvent molecule.

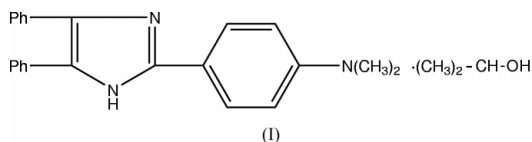
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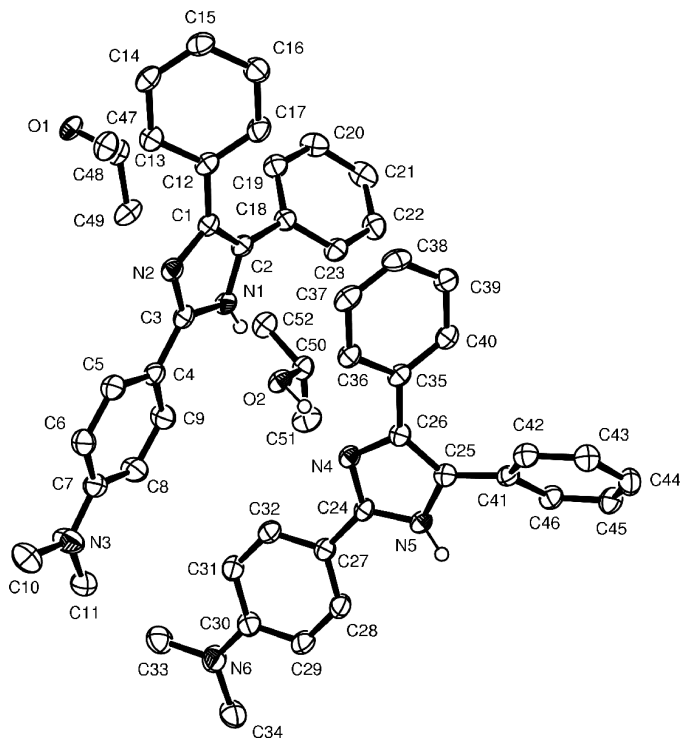
Microwave-assisted organic synthesis (MAOS) has been used extensively since the mid-1990s due to the availability of commercial microwave equipment and the continuing development of solvent-free reaction techniques. Different types of organic compounds have been synthesized using MAOS (Lidström *et al.*, 2001). Usyatinsky & Khmel'nitsky (2000) have reported the use of this technique in the preparation of 2,4,5-substituted imidazoles. Their synthetic procedure involved the condensation of 1,2-diaryethandienones with aldehydes and ammonium acetate as the source of ammonia with an acidic support (acidic silica) in a microwave oven. We attempted to synthesize 2-[4-(dimethylamino)phenyl]-4,5-diphenyl-1H-imidazole using a similar technique in the absence of the acidic support media. Recrystallization of the reaction product from isopropanol afforded compound (I), as shown by single-crystal X-ray structure determination.



Compound (I) crystallizes with two independent molecules, *A* and *B* (Fig. 1), as well as two solvent molecules, in the asymmetric unit. The general conformation of the two molecules is similar, as shown by the dihedral angles between the imidazole ring (C1 to N2 and C26 to N4, ring 1) and the three benzene rings (C4–C9 and C27–C32, ring 2; C12–C17 and C35–C40, ring 3; C18–C23 and C41–C46, ring 4). In molecule *A*, $1/2 = 7.42^\circ$, $1/3 = 36.71^\circ$ and $1/4 = 45.49^\circ$; in molecule *B*, $1/2 = 8.79^\circ$, $1/3 = 40.34^\circ$ and $1/4 = 43.84^\circ$.

A comparison of the bond distances of the imidazole ring of (I) (Table 1) and the mean values of the distances found in similar structures reported in the Cambridge Structural Database (Version 5.25 of October 2003; Allen, 2002) shows that the bond distance N1–C2 (N5–C25 for molecule *B*) is 0.010 Å smaller, the rest of the bond distances being practically the same.

In the crystal structure, the molecules are connected through hydrogen bonds (Table 2) between the NH group of


Figure 1

The molecular structure of (I), showing the atom labelling and 50% probability ellipsoids. H atoms have been omitted for clarity, except for the H atom of the NH group and the solvent OH group. Molecule *A* is on the left and molecule *B* is on the right.

the imidazole ring and the O atom of the isopropanol solvent molecule and between the N atom of the imidazole ring and the OH group of the isopropanol solvent molecule. There are short contacts between C9—H9 and O2 and between C28—H28 and O1($x - 1, y + 1, z$).

Experimental

A mixture of 0.525 g (2.5 mmol) of benzil, 0.372 g (2.5 mmol) of dimethylaminobenzaldehyde and 7 g of ammonium acetate was irradiated with a microwave power of 262 W for 10 min. The reaction product was treated with 20 ml of diethyl ether and filtered. The solid residue was crystallized from isopropanol (m.p. 530–531 K).

Crystal data

$C_{23}H_{21}N_3 \cdot C_3H_8O$
 $M_r = 399.52$
 Triclinic, $P\bar{1}$
 $a = 8.764$ (12) Å
 $b = 12.087$ (14) Å
 $c = 21.07$ (4) Å
 $\alpha = 97.48$ (9)°
 $\beta = 93.12$ (10)°
 $\gamma = 91.89$ (10)°
 $V = 2208$ (6) Å³

$Z = 4$
 $D_x = 1.202$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1567 reflections
 $\theta = 2.6$ – 25.4 °
 $\mu = 0.07$ mm⁻¹
 $T = 393$ (2) K
 Plate, colourless
 $0.45 \times 0.24 \times 0.02$ mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
 ω scans
 Absorption correction: none
 15473 measured reflections
 8644 independent reflections

5245 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.057$
 $\theta_{max} = 26.0$ °
 $h = -8 \rightarrow 10$
 $k = -14 \rightarrow 14$
 $l = -25 \rightarrow 25$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.119$
 $S = 0.85$
 8644 reflections
 565 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0679P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.23$ e Å⁻³
 $\Delta\rho_{min} = -0.25$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—C3	1.362 (3)	N4—C26	1.379 (3)
N1—C2	1.370 (3)	N5—C24	1.361 (3)
N2—C3	1.326 (3)	N5—C25	1.369 (3)
N2—C1	1.379 (3)	C1—C2	1.384 (3)
N4—C24	1.333 (3)	C25—C26	1.381 (3)
C3—N1—C2	108.75 (19)	N1—C2—C1	104.56 (19)
C3—N2—C1	105.67 (18)	N2—C3—N1	110.58 (19)
C24—N4—C26	104.97 (18)	N4—C24—N5	111.13 (19)
C24—N5—C25	108.19 (19)	N5—C25—C26	105.01 (19)
N2—C1—C2	110.44 (18)	N4—C26—C25	110.69 (17)

Table 2

Hydrogen-bonding 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...O2	0.85 (2)	1.95 (2)	2.797 (4)	173 (2)
N5—H2...O1 ⁱ	0.92 (2)	1.92 (2)	2.840 (4)	173 (2)
O1—H3...N2 ⁱⁱ	0.84 (3)	1.97 (3)	2.814 (4)	174 (2)
O2—H4...N4	0.95 (3)	1.86 (3)	2.814 (4)	176 (2)
C9—H9...O2	0.93	2.47	3.329 (7)	155
C28—H28...O1 ⁱ	0.93	2.44	3.294 (7)	153

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

All H atoms were placed in ideal positions and refined as riding [C—H = 0.93 Å or 0.96 Å (methyl H atoms); $U(H) = 1.2$ or 1.5 (methyl H atoms) times $U_{eq}(\text{parent atom})$], except for the H atoms linked to the N and O atoms, which were located in difference Fourier maps and refined freely.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-NT* (Bruker, 1998); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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