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# 2-Methyl-1,4,5-triphenyl-1*H*-imidazole

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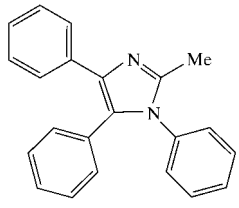
In 2-methyl-1,4,5-triphenyl-1*H*-imidazole, $C_{22}H_{18}N_2$, the three substituent phenyl groups are not delocalized with the imidazole moiety; the dihedral angles these phenyl groups form with the imidazole ring are in the range 25.90 (5)–63.49 (6)°.

## Comment

During the synthesis of a large series of chiral $\alpha$-diimines by condensation of $\alpha$-diketones with chiral primary amines following a known procedure (Mehrotra & Singh, 1980), we obtained the title compound, (I), as an unexpected by-product (see *Experimental*).




(I)

Compound (I) (Table 1, Fig. 1) is a tetrasubstituted imidazole. The imidazole ring presents the common aromatic geometry, with delocalized C···N and C···C $\pi$ bond lengths in the range 1.3123 (16)–1.3950 (16) Å. Due to the substitution at N1, no tautomeric forms are possible for the imidazole moiety, in the solid state or in solution.

The phenyl groups bonded to atoms N1, C4 and C5 are not delocalized with the imidazole ring; the dihedral angles between the least-squares planes of the imidazole and phenyl rings are 63.49 (6), 25.90 (5) and 58.75 (6)° for the C6–C11, C13–C18 and C19–C24 rings, respectively. This relative conformation for the phenyl rings seems to minimize steric hindrance in the overall molecule. A similar non-conjugated arrangement was previously observed for a symmetrically tetrasubstituted imidazole (Buttke *et al.*, 1997). In this case, the substituents on N1, C2, C4 and C5 were 4-methoxyphenyl groups, and the calculated dihedral angles between the phenyl moieties and the imidazole ring were 105.9 (substituent on N1), 15.1 (substituent on C2), 47.9 (substituent on C4) and 101.9° (substituent on C5). Thus, with respect to (I), a significantly different conformation is observed for the groups bonded to the imidazole core. However, it cannot be determined whether these variations are related to the fact that (I) is a non-symmetrical substituted imidazole or result from stacking effects in the solid state.

The fourth substituent in (I) is a methyl group bonded to C2, which has the methyl H atoms disordered over two orientations. Two of the shorter intramolecular contacts involve atom H12*D* of the minor disorder component and a neighbouring phenyl ring on N1 (intramolecular contact distances are C6···H12*D* 2.64 Å and C7···H12*D* 2.61 Å). Such contacts may not exist in solution, but if they do, they are weak enough to allow free rotation of the methyl group in solution at room temperature, in agreement with the sharp singlet observed in NMR for these H atoms at $\delta$ 2.35 p.p.m. (200 MHz, $CDCl_3$).

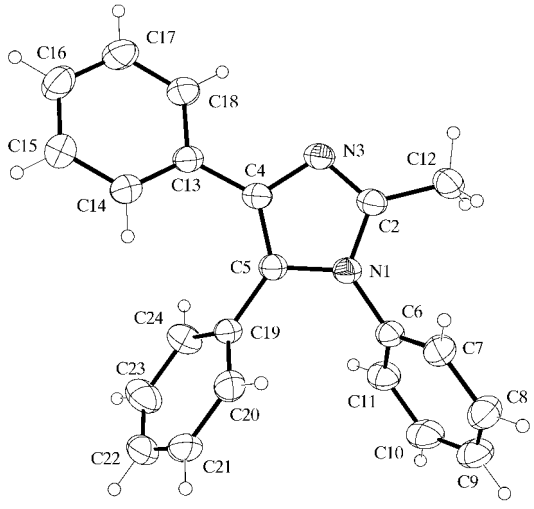



**Figure 1**
The structure of (I), with displacement ellipsoids at the 30% probability level. H atoms are shown as small spheres of arbitrary radii. For the C12-methyl group, the H atoms corresponding to the minor component of the disorder have been omitted.

The packing of the molecule of (I) in the solid state is determined by the low Laue symmetry and the above-mentioned conformation of the phenyl groups. These two features prevent any significant stacking intermolecular interactions in the cell; the shortest interaction between rings is 4.26 Å, for two symmetry-related imidazole rings (symmetry code: $1-x, 1-y, 1-z$). On the other hand, the lack of suitable donor groups for hydrogen bonding favours the separation of the molecules in the cell. The shortest observed intermolecular contact is through the non-substituted imidazole N atom, *viz.* C7—H7···N3$^{i}$ [symmetry code: (i) $1-x, 1-y, 1-z$], with a long H···N contact distance of 2.58 Å and a contact angle of 167°. A consequence of this packing structure is a relatively low packing index (Spek, 1998) of 66.1% for this small molecule.

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## Experimental

Benzil (0.5 g., 2.38 mmol) was reacted with (*S*)-(−)-α-methylbenzylamine (0.7 ml, 5.2 mmol) under an inert atmosphere at 423 K for 30 min. The crude product was extracted with hexane–water (50:50), filtered over $Na_2SO_4$, reduced by evaporation and purified by chromatography [$Al_2O_3$, 150 mesh, hexane–AcOEt (95:5)], yielding four compounds, namely 2,3,5,6-tetraphenylpyrazine, 2,4,5-triphenyl-1*H*-imidazole, 2-methyl-1,4,5-triphenyl-2,3-dihydro-1*H*-imidazole and (I) (respective yields: 25, 20, 15 and 30%). This last compound was crystallized from petroleum ether–EtOH (67:33).

*Crystal data*

$C_{22}H_{18}N_2$
$M_r = 310.38$
Triclinic, $P\overline{1}$
$a = 8.5768\ (5)$ Å
$b = 9.8285\ (9)$ Å
$c = 10.7315\ (7)$ Å
$\alpha = 96.288\ (6)^\circ$
$\beta = 92.042\ (4)^\circ$
$\gamma = 106.338\ (5)^\circ$
$V = 860.79\ (11)$ Å$^3$
$Z = 2$
$D_x = 1.198$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 78 reflections
$\theta = 4.5$–$15.0^\circ$
$\mu = 0.07$ mm$^{-1}$
$T = 299\ (1)$ K
Regular prism, colourless
0.65 × 0.65 × 0.36 mm

*Data collection*

Bruker *P*4 diffractometer
$\omega$ scans
5916 measured reflections
4985 independent reflections
3642 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 30^\circ$
$h = -1 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$
3 standard reflections every 97 reflections
intensity decay: 2%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.145$
$S = 1.04$
4985 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.1152P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.034 (4)

The disordered H atoms bonded to atom C12 were found in difference maps and their site-occupancy factors (SOFs) refined in two parts, with the sum of the SOFs for the two disordered components constrained to 1. The remaining H atoms, bonded to $sp^2$-hybridized C atoms, were placed at idealized positions, with constrained C—H distances of 0.96 Å for methyl and 0.93 Å for aryl H atoms. In the final cycles, all H atoms were constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}$(parent), where $x = 1.5$ for methyl H atoms and 1.2 for all others.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXL*97.

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

| | | | |
|---|---|---|---|
| N1—C2 | 1.3732 (15) | N3—C4 | 1.3900 (15) |
| N1—C5 | 1.3950 (16) | C4—C5 | 1.3754 (15) |
| N1—C6 | 1.4368 (15) | C4—C13 | 1.4721 (17) |
| C2—N3 | 1.3123 (16) | C5—C19 | 1.4787 (16) |
| C2—C12 | 1.4874 (18) | | |
| C2—N1—C5 | 107.14 (10) | C5—C4—N3 | 109.98 (11) |
| C2—N1—C6 | 125.99 (10) | C5—C4—C13 | 130.35 (11) |
| C5—N1—C6 | 126.87 (10) | N3—C4—C13 | 119.44 (10) |
| N3—C2—N1 | 111.36 (11) | C4—C5—N1 | 105.28 (10) |
| N3—C2—C12 | 124.87 (11) | C4—C5—C19 | 132.45 (11) |
| N1—C2—C12 | 123.75 (11) | N1—C5—C19 | 122.27 (10) |
| C2—N3—C4 | 106.25 (10) | | |

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1661). Services for accessing these data are described at the back of the journal.

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