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# 2-Isopropylamino-1-phenyl-1*H*-imidazol-5(4*H*)-one

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The title compound, $C_{12}H_{15}N_3O$, crystallizes with four independent molecules in the asymmetric unit. The five-membered heterocyclic rings are essentially planar. The crystal packing is stabilized by intra- and intermolecular hydrogen bonds and $\pi$–$\pi$ stacking interactions.

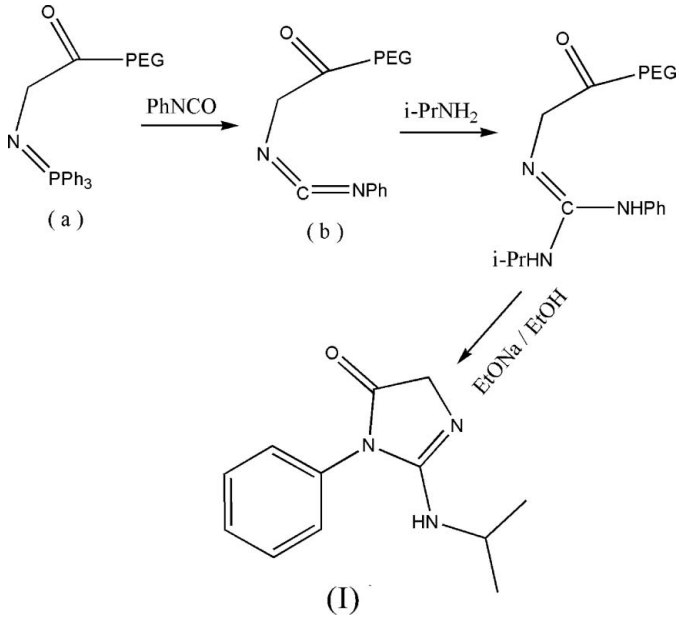
**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.058
$wR$ factor = 0.139
Data-to-parameter ratio = 9.6

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

## Comment

Some compounds belonging to the class of substituted 4*H*-imidazol-4-ones have shown biological and pharmaceutical activities (Sulkowski *et al.*, 1997; Khodair *et al.*, 1998), such as good antibacterial, antifungal and angiotensin antagonist activities (Kiec-Kononowicz *et al.*, 1998; Okazaki *et al.*, 1998; Trivedi *et al.*, 2002). With the aim of obtaining a new precursor of bioactive molecules, the title compound, (I), has been synthesized and its crystal structure is reported here.




The asymmetric unit of (I) consists of four independent molecules (Fig. 1). All the five-membered heterocyclic rings are planar within 0.031 (4) Å. The dihedral angles formed by the C1–C6, C13–C18, C25–C30 and C37–C42 phenyl rings with the attached N1/N2/C7–C9, N4/N5/C19–C21, N7/N8/C31–C33 and N10/N11/C43–C45 imidazole rings are 51.72 (12), 61.71 (14), 50.26 (11) and 55.98 (13)°, respectively.

The crystal structure is stabilized by a complex network of intra- and intermolecular C—H···O and N—H···N hydrogen-bonding interactions (Table 1), linking the molecules into zigzag chains extending along the *a* axis (Fig. 2).

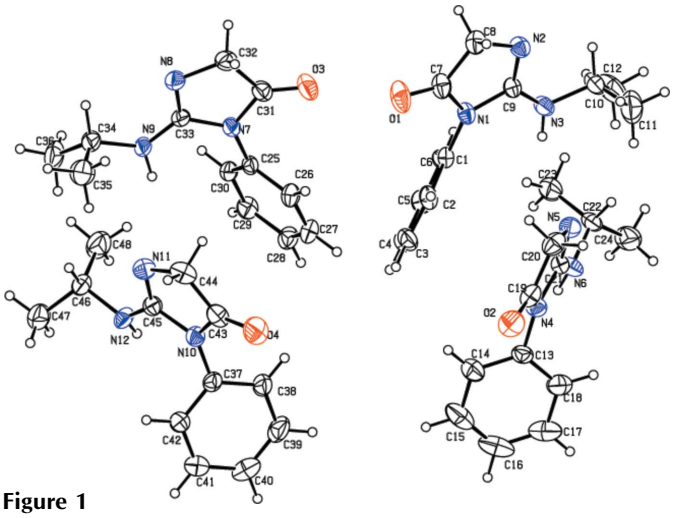


**Figure 1**
The structure of the four independent molecules in the asymmetric unit of compound (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

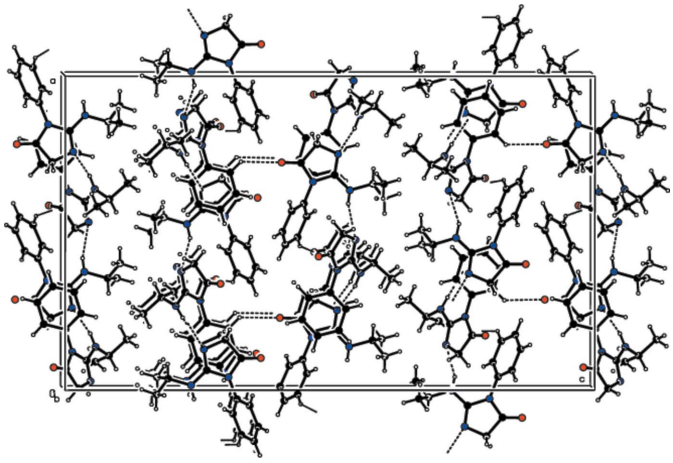


**Figure 2**
Packing diagram of (I), viewed along the *b* axis, showing the formation of intermolecular hydrogen bonds (dashed lines) and $\pi$–$\pi$ stacking interactions.

The crystal structure is further stabilized by $\pi$–$\pi$ stacking interactions involving all the imidazole and phenyl rings, with centroid–centroid separations of 3.760 (7), 3.749 (6), 3.756 (6) and 3.770 (6) Å for $Cg1\cdots Cg6^{i}$, $Cg2\cdots Cg5$, $Cg3\cdots Cg8^{ii}$ and $Cg4\cdots Cg7$, respectively [$Cg1$, $Cg2$ $Cg3$ and $Cg4$ are the centroids of the N1/N2/C7–C9, N4/N5/C19–C21, N7/N8/C31–C33 and N10/N11/C43–C45 imidazole rings, respectively; $Cg5$, $Cg6$, $Cg7$ and $Cg8$ are the centroids of the C1–C6, C13–C18, C25–C30 and C37–C42 phenyl rings, respectively; symmetry codes: (i) $\frac{1}{2}+x, 1-y, z$; (ii) $\frac{1}{2}+x, -y, z$].

## Experimental

To a solution of iminophosphorane (*a*) (3 mmol) in anhydrous dichloromethane (15 ml) was added phenyl isocyanate (3 mmol) under dry nitrogen at room temperature. The reaction mixture was left unstirred for 12 h at 278 K and then the solvent was removed under reduced pressure and diethyl ether/petroleum ether (1:3 *v*/*v*, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, the solvent was removed to give carbodiimide (*b*), which was used directly without further purification. To the solution of the carbodiimide, prepared as above, was added diisopropylamine (3 mmol) in dichloromethane (15 ml). After the reaction mixture had been allowed to stand for 0.5 h, the solvent was removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 3 h at room temperature. The solution was concentrated under reduced pressure and the residue was recrystallized from ethanol to give the title compound, (I), in 82% yield (m.p. 355 K). Elemental analysis calculated for $C_{12}H_{15}N_3O$: C 66.34, H 6.96, N 19.34%; found: C 66.23, H 4.91, N, 19.17%. Crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation of a hexane/dichloromethane solution (1:3 *v*/*v*) at room temperature.

### *Crystal data*

$C_{12}H_{15}N_3O$
$M_r$ = 217.27
Orthorhombic, $Pca2_1$
$a$ = 19.076 (3) Å
$b$ = 7.6881 (10) Å
$c$ = 32.241 (4) Å
$V$ = 4728.4 (11) Å$^3$
$Z$ = 16
$D_x$ = 1.221 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 298 (2) K
Block, colorless
0.30 × 0.20 × 0.20 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
34935 measured reflections
5719 independent reflections
4528 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044
$\theta_{max}$ = 28.0°

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.139
$S$ = 1.10
5719 reflections
597 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2 + 0.2788P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N9—H9···N11 | 0.90 (4) | 2.43 (4) | 3.222 (4) | 148 (3) |
| N3—H3$A$···N5 | 0.84 (4) | 2.52 (4) | 3.312 (4) | 157 (4) |
| C29—H29···O4$^{i}$ | 0.93 | 2.41 | 3.175 (4) | 140 |
| C5—H5···O2$^{i}$ | 0.93 | 2.58 | 3.421 (5) | 151 |
| N12—H12···N8$^{ii}$ | 0.85 (4) | 2.20 (4) | 3.039 (4) | 169 (4) |
| C38—H38···O1$^{iii}$ | 0.93 | 2.48 | 3.203 (5) | 134 |
| N6—H6$A$···N2$^{iii}$ | 0.87 (4) | 2.26 (4) | 3.063 (4) | 153 (4) |

Symmetry codes: (i) $x, y-1, z$; (ii) $x-\frac{1}{2}, -y, z$; (iii) $x-\frac{1}{2}, -y+1, z$.

The H atoms attached to N atoms were located in a difference Fourier map and refined freely. All other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic), 0.96 (methyl) or 0.97 Å (methylene), and included in the refinement in the riding-model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(C) for the methyl H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged in the final refinement.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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