Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 5-Amino-1-phenyl-1*H*-pyrazole

**Zdeněk Trávníček,[a,b]* Jaromír Marek[a,c] and Petr Cankař[d]**

[a]Department of Inorganic Chemistry, Faculty of Science, Palacký University, Křížkovského 10, CZ-771 47 Olomouc, Czech Republic, [b]Laboratory of Growth Regulators, Palacký University, and Institute of Experimental Botany, AS CR, Palacký University, Šlechtitelu 11, CZ-783 71 Olomouc, Czech Republic, [c]Department of Functional Genomics and Proteomics, Faculty of Science, Masaryk University, Kamenice 5, CZ-625 00 Brno, Czech Republic, and [d]Department of Organic Chemistry, Faculty of Science, Palacký University, Tř. Svobody 8, CZ-771 46 Olomouc, Czech Republic

Correspondence e-mail: trav@aix.upol.cz

**Key indicators**

Single-crystal X-ray study
*T* = 105 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.052
*wR* factor = 0.150
Data-to-parameter ratio = 13.3

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

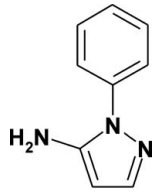


Received 16 January 2006
Accepted 24 January 2006

The structure of the title compound, $C_9H_9N_3$, consists of discrete molecules. The secondary structure is formed by molecules linked by N—H···N hydrogen bonds into linear chains. In addition to the conventional hydrogen bonds, there are several weak interactions of the type N—H···C, and $\pi$ stacking interactions of the type C—H···C.

## Comment

As detailed in the preceding paper (Marek *et al.*, 2006), *N*-phenylpyrazole derivatives have been employed for decades in many branches of chemistry. Moreover, the title compound, (I), may be used a precursor for the preparation of sulfaphenazol (Schmidt & Druey, 1958), a sulfonamide with an antibacterial chemotherapeutic effect, or as an important fragment of selective inhibitors of the mitogen-activated protein (MAP) kinase p38 potentially useful for the treatment of arthritis and osteoporosis (Dumas *et al.*, 2000). This fragment was also used for research of inhibitors of the cysteine protease, cathepsin K (Tavares *et al.*, 2004).




(I)

The molecular structure of (I) is depicted in Fig. 1, and selected bond distances and angles are given in Table 1. Both the rings are slightly deformed. The maximum deviation from the phenyl ring is 0.017 (2) Å for atom C7 and the maximum deviation from the pyrazole ring is 0.010 (2) Å for atom C5. The Cremer–Pople puckering parameters (Cremer & Pople, 1975) for the rings of (I) are $Q$ = 0.028 (2) Å, Θ = 79 (4)° and $\varphi_2$ = 41 (4)° for the phenyl ring and $Q$ = 0.014 (2) Å and $\varphi_2$ = 157 (8)° for the pyrazole ring. These values indicate slight screw-boat deformation of the six-membered and slight half-chair deformation of the five-membered rings. The dihedral angle between the mean planes through the phenyl and pyrazole rings is 37.97 (7)°.

Bond distances and angles are consistent with standard values. Moreover, they are very similar to those found for 1-phenyl-3-aminopyrazole (Marek *et al.*, 2006). The small discrepancies are caused by a different location of the amino group on the pyrazole ring.

In the crystal structure of (I), the secondary structure is formed by molecules linked by N—H···N hydrogen bonds

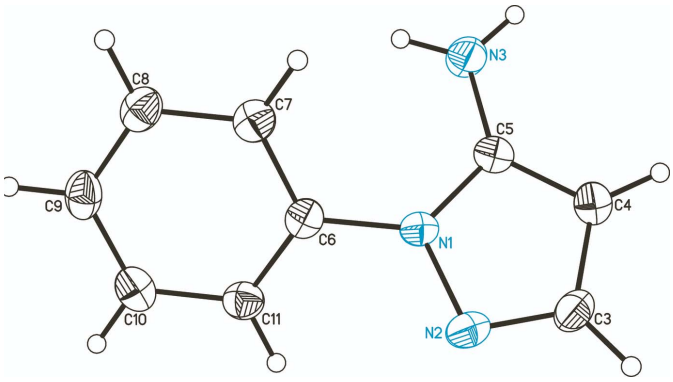



**Figure 1**
A view of the molecular structure of (I). Non-H atoms are drawn with 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii.

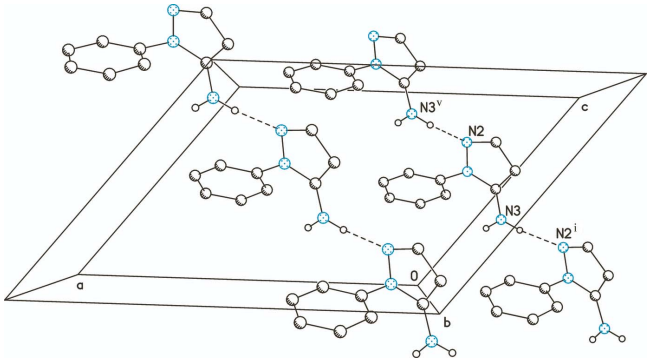



**Figure 2**
Part of the crystal structure of (I), showing the formation of linear chains of hydrogen-bonded (dashed lines) molecules in the [101] direction. [Symmetry codes: (i) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (v) $x+\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2}$]. C-bound H atoms have been omitted for clarity.

into linear chains in the [101] direction (Fig. 2). In addition to the conventional hydrogen bonds, there are several weak interactions of the type N—H···C, and $\pi$ stacking interactions of the type C—H···C (Table 2).

## Experimental

1-Phenyl-5-aminopyrazole, (I), was obtained according to the method described previously (Schmidt & Druey, 1958). The final product was purified by flash chromatography. To obtain crystals suitable for single-crystal X-ray analysis, the solid compound was sublimed in a test-tube with a cooling finger in a vacuum [343 K (oil bath), 1.3 h Pa].

*Crystal data*

$C_9H_9N_3$
$M_r$ = 159.19
Monoclinic, $C2/c$
$a$ = 14.386 (3) Å
$b$ = 14.056 (3) Å
$c$ = 10.462 (2) Å
$\beta$ = 128.97 (3)°
$V$ = 1644.8 (9) Å$^3$
$Z$ = 8
$D_x$ = 1.286 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1962 reflections
$\theta$ = 2.3–26.6°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 105 (2) K
Prism, colorless
0.35 × 0.30 × 0.30 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer
$\omega$ scans
Absorption correction: none
6395 measured reflections
1447 independent reflections
1289 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 25.0°
$h = -13 \rightarrow 17$
$k = -16 \rightarrow 16$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.150
$S$ = 1.24
1447 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| N1—C5 | 1.368 (2) | N3—C5 | 1.377 (3) |
| N1—N2 | 1.383 (2) | C3—C4 | 1.393 (3) |
| N1—C6 | 1.423 (2) | C4—C5 | 1.372 (3) |
| N2—C3 | 1.324 (3) | | |
| C5—N1—N2 | 111.16 (15) | C5—C4—C3 | 105.17 (17) |
| C5—N1—C6 | 128.91 (16) | N1—C5—C4 | 106.80 (17) |
| N2—N1—C6 | 119.87 (15) | N1—C5—N3 | 122.91 (17) |
| C3—N2—N1 | 103.94 (15) | C4—C5—N3 | 130.21 (17) |
| N2—C3—C4 | 112.89 (17) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$B$···N2$^{i}$ | 0.88 | 2.21 | 3.028 (2) | 155 |
| C8—H8···C3$^{ii}$ | 0.95 | 2.85 | 3.695 (3) | 149 |
| C3—H3$C$···C8$^{iii}$ | 0.95 | 2.84 | 3.759 (3) | 162 |
| N3—H3$A$···C7$^{iv}$ | 0.88 | 2.74 | 3.475 (3) | 142 |

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, -y, z-\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, y, -z+\frac{1}{2}$.

H atoms were positioned geometrically, with C—H distances of 0.95 Å and N—H distances of 0.88 Å, and with $U_{iso}$(H) values of $1.2U_{eq}$(C,N).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Johnson & Burnett, 1996); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

Financial support of this work by The Ministry of Education, Youth and Sports of the Czech Republic (MSM6198959218 and MSM6198959216) is gratefully acknowledged.

## References

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Dumas, J., Mokdad, H. H., Sibley, R., Riedl, B., Scott, W. J., Monahan, M. K., Lowinger, T. B., Brennan, C., Natero, R., Turner, T., Johnson, J. S.,

Schoenleber, R., Bhargava, A., Wilhelm, S. M., Housley, T. J., Ranges, G. E. & Shrikhande, A. (2000). *Bioorg. Med. Chem. Lett.* **10**, 2051–2054.
Johnson, C. K. & Burnett, M. N. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Marek, J., Trávníček, Z. & Cankař, P. (2006). *Acta Cryst.* E**61**, **HG6296**.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Oxford Diffraction (2002). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Schmidt, P. & Druey, J. (1958). *Helv. Chim. Acta*, **41**, 306–309.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Tavares, F. X., Deaton, D. N., Miller, A. B., Miller, L. R., Wright, L. L. & Zhou, H. Q. (2004). *J. Med. Chem.* **47**, 5049–5056.