research communications

Crystallographic and spectroscopic characterization of two 1-phenyl-1*H*-imidazoles: 4-(1*H*-imidazol-1-yl)benzaldehyde and 1-(4-methoxyphenyl)-1*H*-imidazole

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The title compounds, $C_{10}H_8N_2O$, (I), and $C_{10}H_{10}N_2O$, (II), are two 1-phenyl-1*H*-imidazole derivatives, which differ in the substituent *para* to the imidazole group on the arene ring, *i.e.* a benzaldehyde, (I), and an anisole, (II). Both molecules pack with different motifs *via* similar weak C—H⋯N/O interactions and differ with respect to the angles between the mean planes of the imidazole and arene rings [24.58 (7)° in (I) and 43.67 (4)° in (II)].

1. Chemical context

N-Arylated imidazoles are commonly found in the structures of an array of biologically active compounds (Ananthu *et al.*, 2021). They have a variety of applications in the medicinal chemistry field, such as use in anticancer and anti-inflammatory medications and as antiviral agents (Shalini *et al.*, 2010). They are also used in agriculture as fungicides, herbicides, and plant-growth regulators (Emel'yanenko *et al.*, 2017). 4-(1*H*-Imidazol-1-yl)benzaldehyde, (I), may be synthesized in high yield by treating 4-bromobenzaldehyde with imidazole in an aprotic solvent with the addition of potassium carbonate and a copper(I) catalyst (Xi *et al.*, 2008). The yellow solid is a common reagent in the synthesis of various targets with antifungal and antibacterial activity. It has been shown that (I) could be used to synthesize a series of 3-[4-(1*H*-imidazol-1-yl)phenyl]prop-2-en-1-ones with antifungal, antioxidant, and antileishmanial activities (Hussain *et al.*, 2009). Cream-colored 1-(4-methoxyphenyl)-1*H*-imidazole, (II), and other similar compounds have been found to work as catalysts in the catalytic epoxidation of olefins with moderate to good yields using mild reaction conditions (Schröder *et al.*, 2009). Compound (II) can be synthesized in a 99% isolated yield by allowing imidazole and 4-iodoanisole to react in acetonitrile in the presence of cesium carbonate and a copper(II) catalyst (Milenković *et al.*, 2019).
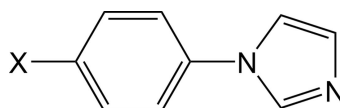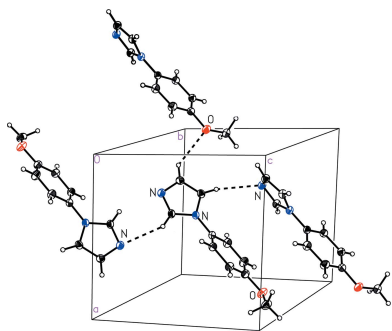
(I) X = C(O)H
(II) X = OCH$_3$

2. Structural commentary

The molecular structures of the benzaldehyde derivative (I) (Fig. 1) and the anisole derivative (II) (Fig. 2) show the *para*

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A···O1[i]	0.95	2.51	3.458 (2)	176
C10—H10A···N2[ii]	0.95	2.51	3.449 (2)	173

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A···N2[i]	0.95	2.55	3.4391 (11)	157
C9—H9A···O1[ii]	0.95	2.56	3.3048 (11)	136
C10—H10A···N2[iii]	0.95	2.52	3.3004 (11)	140

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

nature of the substituent with respect to the imidazole group. The angle between the mean planes of the imidazole and arene rings is 24.58 (7)° in (I) and 43.67 (4)° in (II).

3. Supramolecular features

The molecules of benzaldehyde derivative (I) are held together in the solid state *via* weak C—H···O/N interactions (Fig. 3 and Table 1). Specifically, imidazole C—H groups interact with neighboring benzaldehyde O atoms (C8—H8A···O1[i]) and imidazole N atoms (C10—H10A···N2[ii]). The molecules also stack with an offset face-to-face geometrical arrangement of the arene rings, with an intermolecular centroid-to-centroid distance of 3.7749 (2) Å, a plane-to-centroid distance of 3.5002 (10) Å, and a ring shift of 1.414 (3) Å. Fig. 3 displays a di-periodic sheet with a thickness roughly equivalent to the length of the *c* axis, where the imidazoles interact in the interior and the aldehyde substituents extend to the faces. The sheets then stack in the [001] direction. Notably, (I) crystallizes in the space group $P2_1$ and is therefore a polar material in the solid state. Polar organic materials formed by achiral molecules are of interest in crystal engineering, in particular for nonlinear optical materials (Merritt & Tanski, 2018).

Similarly, the molecules of anisole derivative (II) are held together in the solid state *via* weak C—H···O/N interactions (Fig. 4 and Table 2), with the same imidazole C—H groups as (I) interacting with a neighboring anisole O atom (C9—

H9A···O1[ii]) and an imidazole N atom (C10—H10A···N2[iii]). A third weak interaction links the remaining imidazole H atom with the imidazole N atom (C8—H8A···N2[i]). Unlike benzaldehyde derivative (I), anisole derivative (II) does not exhibit any π-stacking geometrical arrangement of the arene rings and the molecules pack centrosymmetrically (Fig. 5).

4. Database survey

The Cambridge Structural Database (CSD; Groom *et al.*, 2016) contains six simple *para-X*-substituted 1-phenyl-1*H*-
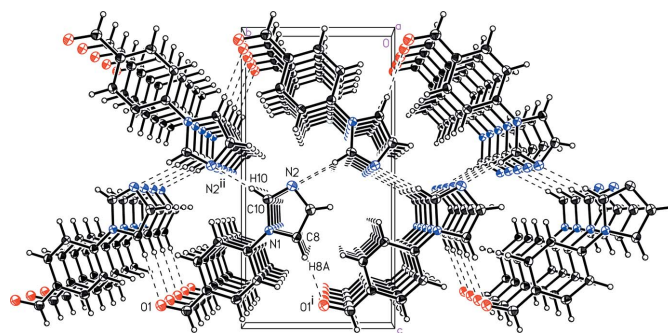
Figure 3
A view of the molecular packing in 4-(1*H*-imidazol-1-yl)benzaldehyde, (I). [Symmetry codes: (i) $x-1, y-1, z$; (ii) $-x+1, y+\frac{1}{2}, -z+1$.]
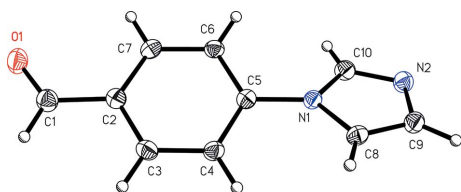

Figure 1
A view of 4-(1*H*-imidazol-1-yl)benzaldehyde, (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.
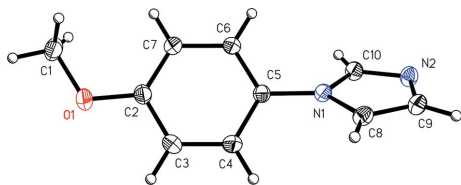

Figure 2
A view of 1-(4-methoxyphenyl)-1*H*-imidazole, (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

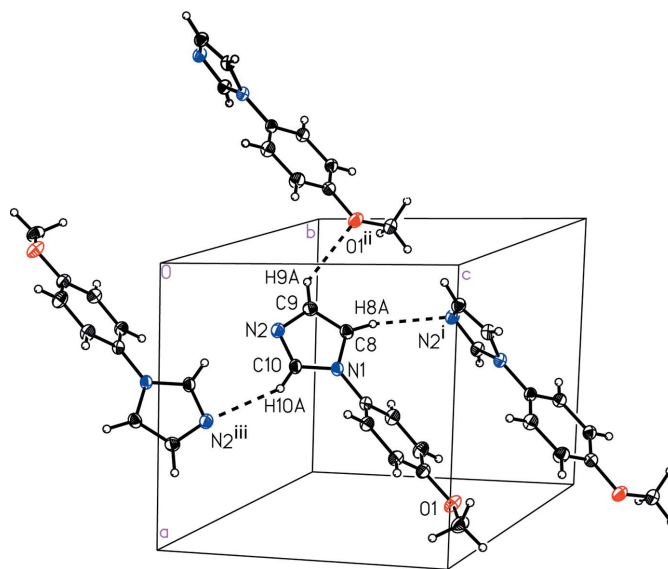**Figure 4**
A view of the intermolecular interactions in 1-(4-methoxyphenyl)-1*H*-imidazole, (II). [Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $x-1, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y+1, -z$.]

Table 3
Experimental details.

Experiments were carried out at 125 K using a Bruker APEXII CCD diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 2016). Refinement was on 119 parameters. H-atom parameters were constrained.

	(I)	(II)
Crystal data		
Chemical formula	$C_{10}H_8N_2O$	$C_{10}H_{10}N_2O$
M_r	172.18	174.20
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1/c$
a, b, c (Å)	3.7749 (2), 7.3711 (5), 14.4524 (9)	8.5663 (12), 11.2143 (16), 9.1635 (13)
β (°)	91.096 (2)	94.448 (2)
V (Å^3)	402.07 (4)	877.6 (2)
Z	2	4
Radiation type	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.77	0.09
Crystal size (mm)	$0.37 \times 0.20 \times 0.05$	$0.40 \times 0.25 \times 0.15$
Data collection		
T_{min}, T_{max}	0.80, 0.96	0.92, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5673, 1482, 1466	21397, 2678, 2332
R_{int}	0.029	0.031
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.615	0.715
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.079, 1.14	0.040, 0.119, 1.04
No. of reflections	1482	2678
No. of restraints	1	0
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.19, −0.15	0.35, −0.29
Absolute structure	Flack x determined using 652 quotients [$(I^+) - (I^-)$]/[$(I^+) + (I^-)$] (Parsons *et al.*, 2013); Hooft y = 0.11(6) calculated with *OLEX2* (Dolomanov *et al.*, 2009)	–
Absolute structure parameter	0.09 (7)	–

Computer programs: *APEX3* and *SAINT* (Bruker, 2013), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2017* (Sheldrick, 2015b), *SHELXTL2014* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009), and *Mercury* (Macrae *et al.*, 2020).

imidazole derivatives: X = –NH$_2$ (CSD refcode MUFCAS; Liang *et al.*, 2009), –Br (PAJDUD; Ding *et al.*, 2021), –I (FIQFUJ; Bejan *et al.*, 2018), –CO$_2$H (IKAWAT; Zheng *et al.*,

Figure 5
A view of the molecular packing in 1-(4-methoxyphenyl)-1*H*-imidazole, (II).

2011), –CO$_2$CH$_3$ (BEMVUN; Khattri *et al.*, 2016) and –COCH$_3$ (XECDUG; Ibrahim *et al.*, 2012). The amino and carboxylic acid derivatives engage in intermolecular hydrogen bonding with the imidazole N atom and exhibit angles between the mean planes of the imidazole and arene rings of 31.17 (MUFCAS) and 14.51° (IKAWAT). The halide derivatives both contain halide to imidazole nitrogen intermolecular contacts and angles between the mean planes of the imidazole and arene rings of 35.22 (PAJDUD) and 27.10° (FIQFUJ). Similar to the title compounds (I) and (II), the methyl ester and methyl ketone derivatives pack *via* weak C—H⋯N/O interactions and with angles between the mean planes of the imidazole and arene rings of 24.83 (BEMVUN) and 1.04° (XECDUG). In XECDUG, a molecule of water hydrogen bonds to the 1*H*-imidazole H and *ortho*-phenyl H of a neighboring molecule, holding the planes of the imidazole and arene rings nearly coplanar. Inspection of the bond lengths of the imidazole ring for all eight derivatives reveals that they are remarkably similar.

5. Synthesis and crystallization

4-(1*H*-Imidazol-1-yl)benzaldehyde (98%), (I), and 1-(4-methoxyphenyl)-1*H*-imidazole (98%), (II), were purchased from Aldrich Chemical Company, USA, and were used as received.
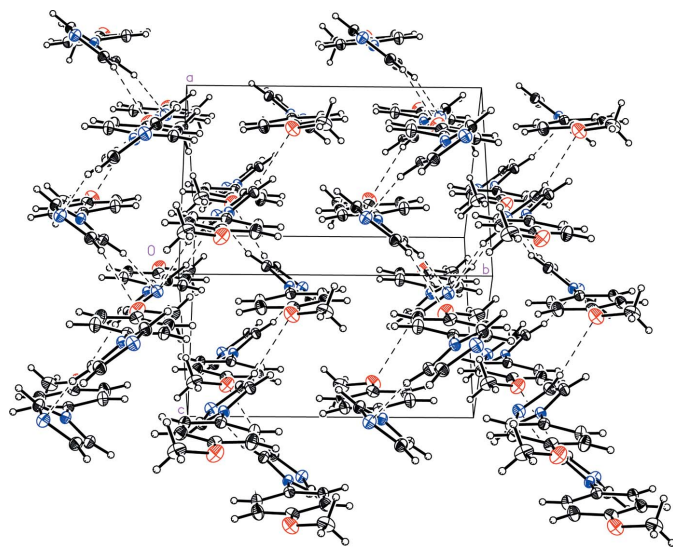
6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms on C atoms were included in calculated positions and refined using a riding model, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl H atoms, and C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms.

7. Analytical data

7.1. 4-(1*H*-Imidazol-1-yl)benzaldehyde, (I)

^{1}H NMR (Bruker Avance III HD 400 MHz, CDCl$_3$): δ 7.26 (*m*, 1H, C$_{imid}$*H*), 7.39 (*m*, 1H, C$_{imid}$*H*), 7.60 (*d*, 2H, C$_{aryl}$*H*, *J* = 8.6 Hz), 7.99 (*s*, 1H, C$_{imid}$*H*), 8.03 (*d*, 2H, C$_{aryl}$*H*, *J* = 8.6 Hz), 10.05 [*s*, 1H, C(O)*H*]. ^{13}C NMR (^{13}C{^{1}H}, 100.6 MHz, CDCl$_3$): δ 117.54 (*C*$_{imid}$H), 120.97 (*C*$_{aryl}$H), 131.23 (*C*$_{imid}$H), 131.48 (*C*$_{aryl}$H), 134.84 (*C*$_{aryl}$), 135.28 (*C*$_{imid}$H), 141.60 (*C*$_{aryl}$), 190.48 [*C*(O)H]. IR (Thermo Nicolet iS50, ATR, cm^{-1}): 3138 (w, C$_{aryl}$—H str), 3109 (*m*, C$_{aryl}$—H str), 2818 and 2746 (*m*, =C—H aldehyde Fermi doublet str), 1676 (*s*, C=O str), 1604 (*s*, arom. C=C str), 1519 (*s*, arom. C=C str), 1481 (*s*, arom. C=C str), 1439 (*m*), 1400 (*s*), 1375 (*s*), 1310 (*s*), 1268 (*s*), 1220 (*s*), 1171 (*s*), 1120 (*m*), 1105 (*m*), 1059 (*s*), 971 (*m*), 959 (*s*), 902 (*w*), 830 (*s*), 752 (*s*), 692 (*m*), 752 (*s*), 692 (*m*), 648 (*s*), 617 (*m*), 530 (*m*), 513 (*s*), 447 (*m*), 413 (*m*). GC–MS (Agilent Technologies 7890A GC/5975C MS): M^+ = 172 amu.

7.2. 1-(4-Methoxyphenyl)-1*H*-imidazole, (II)

^{1}H NMR (Bruker Avance III HD 400 MHz, CDCl$_3$): δ 3.85 (*s*, 3H, OC*H*$_3$), 6.98 (*d*, 2H, C$_{aryl}$*H*, *J* = 8.9 Hz), 7.20 (*m*, 2H, C$_{imid}$*H*), 7.30 (*d*, 2H, C$_{aryl}$*H*, *J* = 8.9 Hz), 7.78 (*m*, 1H, C$_{imid}$*H*). ^{13}C NMR (^{13}C{^{1}H}, 100.6 MHz, CDCl$_3$): δ 55.56 (O*C*H$_3$), 114.87 (*C*$_{aryl}$H), 118.83 (*C*$_{imid}$H), 123.19 (*C*$_{aryl}$H), 129.97 (*C*$_{aryl}$), 130.68 (*C*$_{imid}$H), 135.89 (*C*$_{imid}$H), 158.92 (*C*$_{aryl}$). IR (Thermo Nicolet iS50, ATR, cm^{-1}): 3128 (*m*, C$_{aryl}$—H str), 3107 (*m*, C$_{aryl}$—H str), 2961 (*w*, C$_{alkyl}$—H str), 2918 (*w*, C$_{alkyl}$—H str), 2838 (*m*, C$_{alkyl}$—H str), 2052 (*w*), 1877 (*w*), 1634 (*w*), 1610 (*m*), 1591 (*w*), 1517 (*s*, arom. C=C str), 1471 (*s*, arom. C=C str), 1459 (*m*), 1447 (*w*), 1332 (*m*), 1321 (*s*), 1302 (*m*), 1267 (*s*), 1256 (*s*), 1241 (*s*), 1192 (*s*), 1173 (*m*), 1109 (*s*), 1100 (*s*), 1061 (*s*), 1029 (*s*), 961 (*m*), 910 (*m*), 873 (*w*), 840 (*s*), 823 (*s*), 798 (*s*), 780 (*s*), 762 (*s*), 664 (*s*), 649 (*s*), 614 (*m*), 539 (*s*), 490 (*m*), 434 (*w*). GC–MS (Agilent Technologies 7890A GC/5975C MS): M^+ = 174 amu.

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References

Ananthu, S., Aneeja, T. & Anilkumar, G. (2021). *ChemistrySelect*, **6**, 9794–9805.

Bejan, D., Bahrin, L. G., Shova, S., Sardaru, M., Clima, L., Nicolescu, A., Marangoci, N., Lozan, V. & Janiak, C. (2018). *Inorg. Chim. Acta*, **482**, 275–283.

Bruker (2013). *SAINT* and *APEX3*. Bruxer AXS Inc., Madison, Wisconsin, USA.

Bruker (2016). *SADABS*. Bruxer AXS Inc., Madison, Wisconsin, USA.

Ding, B., Ma, L., Huang, Z., Ma, X. & Tian, H. (2021). *Sci. Adv.* **7**, eabf9668.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Emel'yanenko, V. N., Kaliner, M., Strassner, T. & Verevkin, S. P. (2017). *Fluid Phase Equilib.* **433**, 40–49.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Hussain, T., Siddiqui, H. L., Zia-ur-Rehman, M., Masoom Yasinzai, M. & Parvez, M. (2009). *Eur. J. Med. Chem.* **44**, 4654–4660.

Ibrahim, H., Bala, M. D. & Omondi, B. (2012). *Acta Cryst.* E**68**, o2305.

Khattri, R. B., Morris, D. L., Davis, C. M., Bilinovich, S. M., Caras, A. J., Panzner, M. J., Debord, M. A. & Leeper, T. C. (2016). *Molecules*, pp. 21.

Liang, L., Li, Z. & Zhou, X. (2009). *Org. Lett.* **11**, 3294–3297.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Merritt, H. & Tanski, J. M. (2018). *J. Chem. Crystallogr.* **48**, 109–116.

Milenković, M. R., Papastavrou, A. T., Radanović, D., Pevec, A., Jagličić, Z., Zlatar, M., Gruden, M., Vougioukalakis, G. C., Turel, I., Anđelković, K. & Čobeljić, B. (2019). *Polyhedron*, **165**, 22–30.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Schröder, K., Enthaler, S., Bitterlich, B., Schulz, T., Spannenberg, A., Tse, M. K., Junge, K. & Beller, M. (2009). *Chem. Eur. J.* **15**, 5471–5481.

Shalini, K., Sharma, P. K. & Kumar, N. (2010). *Der Chem. Sinica*, **1**, 6–47.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Xi, Z., Liu, F., Zhou, Y. & Chen, W. (2008). *Tetrahedron*, **64**, 4254–4259.

Zheng, Z., Geng, W.-Q., Wu, Z.-C. & Zhou, H.-P. (2011). *Acta Cryst.* E**67**, o524.

Crystallographic and spectroscopic characterization of two 1-phenyl-1*H*-imidazoles: 4-(1*H*-imidazol-1-yl)benzaldehyde and 1-(4-methoxyphenyl)-1*H*-imidazole

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Computing details

For both structures, data collection: *APEX3* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *SHELXTL2014* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL2014* (Sheldrick, 2008), OLEX2 (Dolomanov *et al.*, 2009), and *Mercury* (Macrae *et al.*, 2020).

4-(1*H*-Imidazol-1-yl)benzaldehyde (I)

Crystal data

$C_{10}H_8N_2O$	$F(000) = 180$
$M_r = 172.18$	$D_x = 1.422$ Mg m^{-3}
Monoclinic, $P2_1$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 3.7749$ (2) Å	Cell parameters from 5426 reflections
$b = 7.3711$ (5) Å	$\theta = 3.1–71.6°$
$c = 14.4524$ (9) Å	$\mu = 0.77$ mm^{-1}
$\beta = 91.096$ (2)°	$T = 125$ K
$V = 402.07$ (4) Å^3	Plate, clear colourless
$Z = 2$	$0.37 \times 0.20 \times 0.05$ mm

Data collection

Bruker APEXII CCD diffractometer	5673 measured reflections
Radiation source: Cu IuS micro-focus source	1482 independent reflections
Detector resolution: 8.3333 pixels mm^{-1}	1466 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.029$
Absorption correction: multi-scan (SADABS; Bruker, 2016)	$\theta_{max} = 71.6°$, $\theta_{min} = 3.1°$
	$h = -4 \rightarrow 4$
	$k = -8 \rightarrow 7$
$T_{min} = 0.80$, $T_{max} = 0.96$	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	119 parameters
Least-squares matrix: full	1 restraint
$R[F^2 > 2\sigma(F^2)] = 0.027$	Primary atom site location: dual
$wR(F^2) = 0.079$	Secondary atom site location: difference Fourier map
$S = 1.14$	
1482 reflections	

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.0471P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.19$ e Å^{-3}

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: SHELXL2017 (Sheldrick, 2015b)

Extinction coefficient: 0.021 (6)

Absolute structure: Flack x determined using 652 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013); Hooft $y = 0.11(6)$ calculated with OLEX2 (Dolomanov *et al.*, 2009).

Absolute structure parameter: 0.09 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.8970 (4)	0.9617 (2)	0.09534 (10)	0.0289 (4)
N1	0.3041 (4)	0.2861 (2)	0.33233 (10)	0.0166 (4)
N2	0.2148 (4)	0.1490 (2)	0.46723 (11)	0.0222 (4)
C1	0.8366 (5)	0.8021 (3)	0.07934 (13)	0.0230 (4)
H1A	0.889378	0.758391	0.019326	0.028*
C2	0.6890 (5)	0.6719 (3)	0.14516 (12)	0.0185 (4)
C3	0.6418 (5)	0.4920 (3)	0.11753 (13)	0.0203 (4)
H3A	0.698927	0.4571	0.056322	0.024*
C4	0.5120 (5)	0.3631 (3)	0.17851 (12)	0.0192 (4)
H4A	0.480518	0.240754	0.159434	0.023*
C5	0.4286 (4)	0.4165 (3)	0.26824 (12)	0.0169 (4)
C6	0.4704 (4)	0.5971 (3)	0.29652 (12)	0.0183 (4)
H6A	0.409116	0.632564	0.357352	0.022*
C7	0.6015 (5)	0.7236 (3)	0.23531 (13)	0.0199 (4)
H7A	0.632366	0.846022	0.254394	0.024*
C8	0.1451 (4)	0.1207 (3)	0.31214 (12)	0.0191 (4)
H8A	0.086412	0.073743	0.25258	0.023*
C9	0.0906 (5)	0.0395 (3)	0.39529 (13)	0.0212 (4)
H9A	−0.017271	−0.075833	0.403072	0.025*
C10	0.3399 (5)	0.2943 (3)	0.42704 (13)	0.0204 (4)
H10A	0.443164	0.393702	0.45957	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0395 (9)	0.0225 (9)	0.0249 (7)	−0.0053 (6)	0.0026 (6)	0.0022 (6)
N1	0.0195 (7)	0.0148 (9)	0.0154 (7)	0.0001 (6)	−0.0004 (5)	0.0002 (6)
N2	0.0268 (8)	0.0210 (10)	0.0188 (7)	−0.0002 (6)	0.0009 (6)	0.0014 (6)
C1	0.0245 (9)	0.0236 (12)	0.0209 (9)	−0.0008 (8)	−0.0004 (7)	0.0000 (8)
C2	0.0179 (8)	0.0201 (11)	0.0175 (8)	0.0005 (7)	−0.0013 (7)	0.0002 (7)
C3	0.0212 (9)	0.0230 (11)	0.0166 (9)	0.0020 (7)	0.0012 (7)	−0.0018 (7)
C4	0.0230 (9)	0.0166 (11)	0.0180 (8)	−0.0005 (7)	−0.0001 (7)	−0.0021 (7)

C5	0.0151 (8)	0.0176 (10)	0.0180 (8)	0.0009 (7)	−0.0018 (6)	0.0007 (7)
C6	0.0212 (8)	0.0175 (10)	0.0164 (8)	0.0015 (7)	0.0006 (7)	−0.0021 (7)
C7	0.0213 (9)	0.0162 (10)	0.0221 (10)	0.0002 (7)	−0.0015 (7)	−0.0017 (7)
C8	0.0202 (8)	0.0168 (10)	0.0203 (8)	−0.0005 (7)	−0.0009 (6)	−0.0027 (7)
C9	0.0219 (9)	0.0187 (11)	0.0229 (9)	0.0004 (7)	0.0007 (7)	0.0016 (7)
C10	0.0243 (9)	0.0207 (11)	0.0163 (9)	0.0005 (7)	−0.0013 (7)	−0.0012 (7)

Geometric parameters (Å, º)

O1—C1	1.219 (3)	C3—H3A	0.9500
N1—C10	1.374 (2)	C4—C5	1.397 (2)
N1—C8	1.388 (2)	C4—H4A	0.9500
N1—C5	1.421 (2)	C5—C6	1.401 (3)
N2—C10	1.311 (2)	C6—C7	1.383 (3)
N2—C9	1.391 (2)	C6—H6A	0.9500
C1—C2	1.469 (2)	C7—H7A	0.9500
C1—H1A	0.9500	C8—C9	1.362 (3)
C2—C3	1.395 (3)	C8—H8A	0.9500
C2—C7	1.403 (2)	C9—H9A	0.9500
C3—C4	1.391 (3)	C10—H10A	0.9500
C10—N1—C8	106.39 (15)	C4—C5—N1	119.84 (17)
C10—N1—C5	126.28 (15)	C6—C5—N1	119.32 (16)
C8—N1—C5	127.19 (15)	C7—C6—C5	119.59 (17)
C10—N2—C9	105.21 (15)	C7—C6—H6A	120.2
O1—C1—C2	125.41 (17)	C5—C6—H6A	120.2
O1—C1—H1A	117.3	C6—C7—C2	120.28 (18)
C2—C1—H1A	117.3	C6—C7—H7A	119.9
C3—C2—C7	119.54 (17)	C2—C7—H7A	119.9
C3—C2—C1	118.92 (15)	C9—C8—N1	105.83 (16)
C7—C2—C1	121.53 (17)	C9—C8—H8A	127.1
C4—C3—C2	120.81 (16)	N1—C8—H8A	127.1
C4—C3—H3A	119.6	C8—C9—N2	110.49 (18)
C2—C3—H3A	119.6	C8—C9—H9A	124.8
C3—C4—C5	118.95 (17)	N2—C9—H9A	124.8
C3—C4—H4A	120.5	N2—C10—N1	112.07 (16)
C5—C4—H4A	120.5	N2—C10—H10A	124.0
C4—C5—C6	120.84 (16)	N1—C10—H10A	124.0
O1—C1—C2—C3	−178.55 (18)	N1—C5—C6—C7	178.08 (15)
O1—C1—C2—C7	0.2 (3)	C5—C6—C7—C2	0.6 (2)
C7—C2—C3—C4	−0.6 (3)	C3—C2—C7—C6	0.2 (3)
C1—C2—C3—C4	178.21 (16)	C1—C2—C7—C6	−178.52 (16)
C2—C3—C4—C5	0.1 (3)	C10—N1—C8—C9	0.62 (19)
C3—C4—C5—C6	0.7 (3)	C5—N1—C8—C9	176.67 (16)
C3—C4—C5—N1	−178.42 (15)	N1—C8—C9—N2	−0.6 (2)
C10—N1—C5—C4	153.02 (17)	C10—N2—C9—C8	0.4 (2)
C8—N1—C5—C4	−22.3 (2)	C9—N2—C10—N1	0.0 (2)

C10—N1—C5—C6	−26.2 (3)	C8—N1—C10—N2	−0.4 (2)
C8—N1—C5—C6	158.54 (16)	C5—N1—C10—N2	−176.52 (16)
C4—C5—C6—C7	−1.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C8—H8A⋯O1[i]	0.95	2.51	3.458 (2)	176
C10—H10A⋯N2[ii]	0.95	2.51	3.449 (2)	173

Symmetry codes: (i) x−1, y−1, z; (ii) −x+1, y+1/2, −z+1.

1-(4-Methoxyphenyl)-1H-imidazole (II)

Crystal data

$C_{10}H_{10}N_2O$	$F(000) = 368$
$M_r = 174.20$	$D_x = 1.318$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.5663$ (12) Å	Cell parameters from 8588 reflections
$b = 11.2143$ (16) Å	$\theta = 2.4$–30.4°
$c = 9.1635$ (13) Å	$\mu = 0.09$ mm^{-1}
$\beta = 94.448$ (2)°	$T = 125$ K
$V = 877.6$ (2) Å^3	Plate, colourless
$Z = 4$	$0.40 \times 0.25 \times 0.15$ mm

Data collection

Bruker APEXII CCD diffractometer	$T_{min} = 0.92$, $T_{max} = 0.99$
Radiation source: sealed X-ray tube, Bruker APEXII CCD	21397 measured reflections
	2678 independent reflections
Graphite monochromator	2332 reflections with $I > 2\sigma(I)$
Detector resolution: 8.3333 pixels mm^{-1}	$R_{int} = 0.031$
φ and ω scans	$\theta_{max} = 30.6°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (SADABS; Bruker, 2016)	$h = -12 \rightarrow 12$
	$k = -16 \rightarrow 15$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.119$	
$S = 1.04$	H-atom parameters constrained
2678 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 0.1966P]$ where $P = (F_o^2 + 2F_c^2)/3$
119 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: dual	$\Delta\rho_{max} = 0.35$ e Å^{-3}
	$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.50111 (8)	0.64826 (6)	0.27442 (7)	0.01696 (16)
N2	0.35189 (9)	0.60120 (7)	0.07295 (8)	0.02110 (17)
O1	0.98420 (8)	0.63969 (6)	0.71768 (7)	0.02769 (18)
C1	1.02429 (11)	0.53203 (10)	0.79493 (10)	0.0289 (2)
H1A	1.108753	0.547969	0.87077	0.043*
H1B	1.059244	0.472373	0.726426	0.043*
H1C	0.932403	0.501862	0.840608	0.043*
C2	0.86571 (10)	0.63397 (8)	0.60922 (9)	0.02084 (18)
C3	0.81994 (11)	0.74301 (8)	0.54587 (10)	0.02479 (19)
H3A	0.870761	0.814315	0.579384	0.03*
C4	0.70105 (11)	0.74809 (8)	0.43457 (9)	0.02198 (18)
H4A	0.670793	0.822403	0.391376	0.026*
C5	0.62626 (10)	0.64337 (7)	0.38651 (9)	0.01708 (17)
C6	0.67205 (10)	0.53468 (7)	0.44827 (9)	0.01901 (17)
H6A	0.621215	0.463503	0.414318	0.023*
C7	0.79220 (10)	0.52919 (8)	0.55986 (9)	0.02071 (18)
H7A	0.823565	0.454653	0.601777	0.025*
C8	0.37965 (10)	0.72974 (7)	0.26290 (9)	0.01978 (18)
H8A	0.362414	0.793692	0.327719	0.024*
C9	0.28976 (10)	0.69928 (8)	0.13921 (9)	0.02107 (18)
H9A	0.197198	0.739844	0.10349	0.025*
C10	0.47846 (10)	0.57358 (7)	0.15758 (9)	0.01911 (18)
H10A	0.545959	0.509019	0.139087	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0198 (3)	0.0156 (3)	0.0153 (3)	0.0015 (2)	0.0003 (2)	−0.0014 (2)
N2	0.0226 (4)	0.0219 (4)	0.0183 (3)	0.0020 (3)	−0.0011 (3)	−0.0016 (3)
O1	0.0249 (3)	0.0327 (4)	0.0239 (3)	−0.0069 (3)	−0.0077 (3)	0.0039 (3)
C1	0.0249 (4)	0.0389 (5)	0.0222 (4)	−0.0024 (4)	−0.0028 (3)	0.0082 (4)
C2	0.0194 (4)	0.0251 (4)	0.0178 (4)	−0.0035 (3)	0.0003 (3)	0.0010 (3)
C3	0.0271 (4)	0.0204 (4)	0.0260 (4)	−0.0055 (3)	−0.0037 (3)	−0.0010 (3)
C4	0.0264 (4)	0.0162 (4)	0.0228 (4)	−0.0015 (3)	−0.0013 (3)	0.0004 (3)
C5	0.0188 (4)	0.0176 (4)	0.0148 (3)	−0.0004 (3)	0.0009 (3)	−0.0006 (3)
C6	0.0205 (4)	0.0167 (4)	0.0195 (4)	−0.0014 (3)	−0.0001 (3)	−0.0001 (3)
C7	0.0214 (4)	0.0205 (4)	0.0200 (4)	−0.0013 (3)	−0.0001 (3)	0.0031 (3)
C8	0.0231 (4)	0.0166 (4)	0.0197 (4)	0.0034 (3)	0.0024 (3)	−0.0010 (3)
C9	0.0211 (4)	0.0209 (4)	0.0211 (4)	0.0037 (3)	0.0005 (3)	0.0011 (3)
C10	0.0221 (4)	0.0181 (4)	0.0170 (3)	0.0018 (3)	0.0004 (3)	−0.0031 (3)

Geometric parameters (Å, º)

N1—C10	1.3612 (10)	C3—C4	1.3854 (12)
N1—C8	1.3827 (10)	C3—H3A	0.9500

N1—C5	1.4271 (10)	C4—C5	1.3928 (11)
N2—C10	1.3200 (10)	C4—H4A	0.9500
N2—C9	1.3828 (11)	C5—C6	1.3876 (11)
O1—C2	1.3658 (10)	C6—C7	1.3947 (11)
O1—C1	1.4279 (12)	C6—H6A	0.9500
C1—H1A	0.9800	C7—H7A	0.9500
C1—H1B	0.9800	C8—C9	1.3634 (11)
C1—H1C	0.9800	C8—H8A	0.9500
C2—C7	1.3920 (12)	C9—H9A	0.9500
C2—C3	1.3967 (12)	C10—H10A	0.9500
C10—N1—C8	106.62 (7)	C5—C4—H4A	120.3
C10—N1—C5	126.57 (7)	C6—C5—C4	120.21 (8)
C8—N1—C5	126.81 (7)	C6—C5—N1	120.01 (7)
C10—N2—C9	104.78 (7)	C4—C5—N1	119.78 (7)
C2—O1—C1	117.23 (7)	C5—C6—C7	120.46 (7)
O1—C1—H1A	109.5	C5—C6—H6A	119.8
O1—C1—H1B	109.5	C7—C6—H6A	119.8
H1A—C1—H1B	109.5	C2—C7—C6	119.38 (8)
O1—C1—H1C	109.5	C2—C7—H7A	120.3
H1A—C1—H1C	109.5	C6—C7—H7A	120.3
H1B—C1—H1C	109.5	C9—C8—N1	105.73 (7)
O1—C2—C7	124.61 (8)	C9—C8—H8A	127.1
O1—C2—C3	115.48 (8)	N1—C8—H8A	127.1
C7—C2—C3	119.91 (8)	C8—C9—N2	110.64 (7)
C4—C3—C2	120.57 (8)	C8—C9—H9A	124.7
C4—C3—H3A	119.7	N2—C9—H9A	124.7
C2—C3—H3A	119.7	N2—C10—N1	112.23 (7)
C3—C4—C5	119.47 (8)	N2—C10—H10A	123.9
C3—C4—H4A	120.3	N1—C10—H10A	123.9
C1—O1—C2—C7	−6.43 (13)	N1—C5—C6—C7	−178.75 (7)
C1—O1—C2—C3	174.10 (8)	O1—C2—C7—C6	179.88 (8)
O1—C2—C3—C4	179.87 (8)	C3—C2—C7—C6	−0.68 (13)
C7—C2—C3—C4	0.38 (14)	C5—C6—C7—C2	0.19 (13)
C2—C3—C4—C5	0.41 (14)	C10—N1—C8—C9	0.16 (9)
C3—C4—C5—C6	−0.91 (13)	C5—N1—C8—C9	179.98 (7)
C3—C4—C5—N1	178.46 (7)	N1—C8—C9—N2	−0.15 (10)
C10—N1—C5—C6	−44.15 (12)	C10—N2—C9—C8	0.07 (10)
C8—N1—C5—C6	136.07 (9)	C9—N2—C10—N1	0.03 (10)
C10—N1—C5—C4	136.49 (9)	C8—N1—C10—N2	−0.12 (10)
C8—N1—C5—C4	−43.30 (12)	C5—N1—C10—N2	−179.94 (7)
C4—C5—C6—C7	0.61 (13)		

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$A\cdots$N2[i]	0.95	2.55	3.4391 (11)	157

C9—H9A···O1^{ii}	0.95	2.56	3.3048 (11)	136
C10—H10A···N2^{iii}	0.95	2.52	3.3004 (11)	140

Symmetry codes: (i) x, −y+3/2, z+1/2; (ii) x−1, −y+3/2, z−1/2; (iii) −x+1, −y+1, −z.