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2-*p*-Tolyl-4,5-dihydro-1*H*-imidazoleReza Kia,^a Hoong-Kun Fun^{a*} and Hadi Kargar^b

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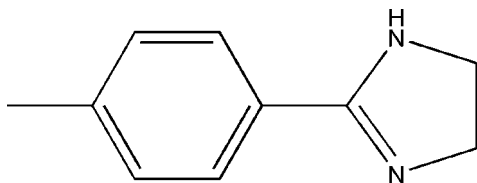
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 12.5.

In the molecule of the title compound, $\text{C}_{10}\text{H}_{12}\text{N}_2$, the six- and five-membered rings are almost co-planar, forming a dihedral angle of 3.56 (8)°. In the crystal structure, neighbouring molecules are linked together by intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds into one-dimensional infinite chains along the c axis. The crystal structure, is further stabilized by weak intermolecular $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ stacking [centroid-centroid distance = 3.8892 (9) Å] interactions.

Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures and syntheses, see: Stibrany *et al.* (2004); Kia *et al.*, 2008, 2009). For applications of imidazoline derivatives, see, for example: Blancafort (1978); Chan (1993); Vizi (1986); Li *et al.* (1996); Ueno *et al.*, (1995); Corey & Grogan (1999). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{12}\text{N}_2$ $V = 850.66$ (3) Å³
 $M_r = 160.22$ $Z = 4$
 Monoclinic, Cc $\text{Mo } K\alpha$ radiation
 $a = 5.1134$ (1) Å $\mu = 0.08$ mm⁻¹
 $b = 16.4020$ (4) Å $T = 100$ K
 $c = 10.1712$ (2) Å $0.47 \times 0.12 \times 0.09$ mm
 $\beta = 94.293$ (1)°

Data collection

Bruker SMART APEXII CCD 8503 measured reflections
 area-detector diffractometer 1423 independent reflections
 Absorption correction: multi-scan 1338 reflections with $I > 2I$
 (SADABS; Bruker, 2005) $R_{\text{int}} = 0.031$
 $T_{\text{min}} = 0.883$, $T_{\text{max}} = 0.993$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$ H atoms treated by a mixture of
 $wR(F^2) = 0.102$ independent and constrained
 $S = 1.08$ refinement
 1423 reflections $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 114 parameters $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³
 2 restraints

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N1}\cdots\text{N2}^{\text{i}}$	0.87 (3)	2.06 (3)	2.9224 (18)	170 (2)
$\text{C10}-\text{H10B}\cdots\text{Cg1}^{\text{ii}}$	0.96	2.88	3.8110 (16)	163

Symmetry codes: (i) $x, -y, z - \frac{1}{2}$; (ii) $x + 1, y, z$. Cg1 is the centroid of the N1/C2/C1/N2/C3 ring.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2738).

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supplementary materials

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2-*p*-Tolyl-4,5-dihydro-1*H*-imidazole

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Comment

Imidazoline derivatives are of great importance because they exhibit significant biological and pharmacological activities such as antihypertensive (Blancafort 1978), antihyperglycemic (Chan 1993), antidepressive (Vizi 1986), antihypercholesterolemic (Li *et al.*, 1996) and antiinflammatory (Ueno *et al.*, 1995). These compounds are also used as catalysts and synthetic intermediates in some organic reactions (Corey & Grogan 1999). With regards to the important applications of imidazolines, herein we report the crystal structure of the title compound, (I).

In the title compound (I, Fig. 1), bond lengths (Allen *et al.* 1987) and angles are within the normal ranges and are comparable with the related structures (Stibrany *et al.* 2004; Kia *et al.*, 2008, 2009). The molecule is almost planar with a maximum deviation from the mean plane of the molecule for C2 atom being -0.176 (19) Å. The six- and five-membered rings are twisted from each other, forming the dihedral angle of 3.56 (8)°. The interesting feature of the crystal structure is the short C2...C10ⁱ contact [3.368 (2) Å; (i) 1 + x, y, z], which is shorter than the sum of the van der Waals radius of carbon atom. In the crystal structure, neighbouring molecules are linked together by intermolecular N—H...N hydrogen bonds into 1-D infinite chains along the *c* axis (Table 1, Fig. 2). The crystal structure is further stabilized by weak intermolecular π - π stacking [*Cg1*...*Cg2*ⁱⁱⁱ = 3.8892 Å; (iii) -1 + x, y, z] and C—H... π interactions (*Cg1* and *Cg2* are the centroids of the N1/C2/C1/N2/C3-imidazoline and the benzene rings, respectively).

Experimental

The synthetic method was based on the previous work (Stibrany *et al.* 2004), except that 10 mmol of 4-methyl cyanobenzene and 40 mmol of ethylenediamine was used. Single crystals suitable for *X*-ray diffraction were obtained by evaporation of a methanol solution at room temperature.

Refinement

The N-bound hydrogen was located from the difference Fourier map and refined freely (see Table. 1). The rest of the hydrogen atoms were positioned geometrically with a riding approximation model with C—H = 0.93–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2$ & 1.5 $U_{\text{eq}}(\text{C})$. A rotating group model was applied for the methyl group. The 1120 Friedel pairs were merged before final refinement as there is not sufficient anomalous dispersion to determine the absolute structure.

Figures

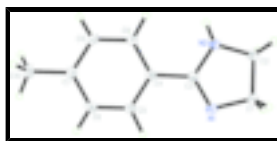


Fig. 1. The molecular structure of (I) with atom labels and 50% probability ellipsoids for non-H atoms.



Fig. 2. The crystal packing of (I), viewed down the *b*-axis showing a 1-D infinite chain along the *c*-axis by intermolecular N—H...N interactions. The intermolecular interactions are shown as dashed lines.

2-*p*-Tolyl-4,5-dihydro-1*H*-imidazole

Crystal data

$C_{10}H_{12}N_2$	$F_{000} = 344$
$M_r = 160.22$	$D_x = 1.251 \text{ Mg m}^{-3}$
Monoclinic, <i>Cc</i>	Mo $K\alpha$ radiation
Hall symbol: C -2yc	$\lambda = 0.71073 \text{ \AA}$
$a = 5.1134 (1) \text{ \AA}$	Cell parameters from 3821 reflections
$b = 16.4020 (4) \text{ \AA}$	$\theta = 2.5\text{--}31.5^\circ$
$c = 10.1712 (2) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 94.293 (1)^\circ$	$T = 100 \text{ K}$
$V = 850.66 (3) \text{ \AA}^3$	Needle, colourless
$Z = 4$	$0.47 \times 0.12 \times 0.09 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	1423 independent reflections
Radiation source: fine-focus sealed tube	1338 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.031$
$T = 100 \text{ K}$	$\theta_{\text{max}} = 31.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.883$, $T_{\text{max}} = 0.993$	$k = -24 \rightarrow 24$
8503 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2 + 0.0868P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
1423 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
114 parameters	$\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N2	-0.2547 (3)	-0.01211 (8)	1.08200 (13)	0.0175 (3)
N1	-0.2444 (3)	-0.02899 (8)	0.86191 (12)	0.0189 (3)
C1	-0.4382 (3)	-0.07930 (9)	1.04580 (15)	0.0190 (3)
H1A	-0.6091	-0.0684	1.0774	0.023*
H1B	-0.3728	-0.1303	1.0837	0.023*
C2	-0.4570 (3)	-0.08371 (9)	0.89368 (15)	0.0181 (3)
H2A	-0.4279	-0.1388	0.8631	0.022*
H2B	-0.6256	-0.0644	0.8561	0.022*
C3	-0.1632 (3)	0.01280 (8)	0.97337 (13)	0.0142 (3)
C4	0.0262 (3)	0.08065 (8)	0.96924 (15)	0.0141 (2)
C5	0.1072 (3)	0.12199 (9)	1.08498 (14)	0.0189 (3)
H5A	0.0404	0.1069	1.1640	0.023*
C6	0.2870 (3)	0.18556 (9)	1.08343 (15)	0.0201 (3)
H6A	0.3393	0.2125	1.1615	0.024*
C7	0.3900 (3)	0.20952 (8)	0.96598 (14)	0.0171 (3)
C8	0.3049 (3)	0.16917 (9)	0.85050 (15)	0.0216 (3)
H8A	0.3690	0.1851	0.7712	0.026*
C9	0.1253 (3)	0.10529 (9)	0.85124 (15)	0.0202 (3)
H9A	0.0712	0.0790	0.7729	0.024*
C10	0.5915 (3)	0.27668 (9)	0.96448 (17)	0.0229 (3)
H10A	0.5467	0.3127	0.8918	0.034*
H10B	0.7613	0.2534	0.9550	0.034*
H10C	0.5946	0.3067	1.0456	0.034*
H1N1	-0.233 (5)	-0.0121 (14)	0.781 (3)	0.031 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0216 (6)	0.0188 (5)	0.0123 (5)	-0.0046 (5)	0.0029 (5)	0.0002 (4)
N1	0.0257 (7)	0.0208 (6)	0.0103 (5)	-0.0085 (5)	0.0011 (5)	-0.0010 (4)

supplementary materials

C1	0.0227 (7)	0.0211 (6)	0.0134 (6)	-0.0059 (5)	0.0035 (5)	0.0005 (5)
C2	0.0201 (7)	0.0197 (6)	0.0145 (6)	-0.0052 (5)	0.0007 (5)	-0.0002 (5)
C3	0.0157 (6)	0.0148 (6)	0.0123 (6)	0.0002 (5)	0.0014 (5)	-0.0002 (4)
C4	0.0156 (6)	0.0147 (5)	0.0118 (5)	-0.0008 (4)	0.0004 (4)	0.0003 (4)
C5	0.0251 (8)	0.0204 (6)	0.0111 (6)	-0.0053 (6)	0.0009 (5)	0.0015 (5)
C6	0.0252 (8)	0.0224 (6)	0.0122 (6)	-0.0067 (6)	-0.0025 (6)	-0.0001 (5)
C7	0.0169 (7)	0.0173 (6)	0.0171 (6)	-0.0031 (5)	0.0011 (5)	0.0012 (5)
C8	0.0260 (8)	0.0233 (7)	0.0164 (6)	-0.0081 (6)	0.0076 (6)	-0.0009 (5)
C9	0.0257 (8)	0.0219 (6)	0.0134 (6)	-0.0074 (6)	0.0048 (5)	-0.0024 (5)
C10	0.0211 (8)	0.0226 (6)	0.0249 (7)	-0.0078 (6)	0.0008 (6)	0.0013 (6)

Geometric parameters (Å, °)

N2—C3	1.2976 (17)	C5—C6	1.391 (2)
N2—C1	1.4763 (19)	C5—H5A	0.9300
N1—C3	1.3627 (17)	C6—C7	1.3975 (19)
N1—C2	1.4641 (19)	C6—H6A	0.9300
N1—H1N1	0.87 (3)	C7—C8	1.389 (2)
C1—C2	1.5447 (19)	C7—C10	1.5092 (19)
C1—H1A	0.9700	C8—C9	1.394 (2)
C1—H1B	0.9700	C8—H8A	0.9300
C2—H2A	0.9700	C9—H9A	0.9300
C2—H2B	0.9700	C10—H10A	0.9600
C3—C4	1.4779 (18)	C10—H10B	0.9600
C4—C5	1.394 (2)	C10—H10C	0.9600
C4—C9	1.397 (2)		
C3—N2—C1	106.60 (12)	C6—C5—C4	120.66 (13)
C3—N1—C2	108.04 (12)	C6—C5—H5A	119.7
C3—N1—H1N1	125.8 (17)	C4—C5—H5A	119.7
C2—N1—H1N1	120.4 (18)	C5—C6—C7	120.80 (13)
N2—C1—C2	105.98 (12)	C5—C6—H6A	119.6
N2—C1—H1A	110.5	C7—C6—H6A	119.6
C2—C1—H1A	110.5	C8—C7—C6	118.33 (13)
N2—C1—H1B	110.5	C8—C7—C10	120.66 (13)
C2—C1—H1B	110.5	C6—C7—C10	121.01 (13)
H1A—C1—H1B	108.7	C7—C8—C9	121.21 (13)
N1—C2—C1	101.59 (11)	C7—C8—H8A	119.4
N1—C2—H2A	111.5	C9—C8—H8A	119.4
C1—C2—H2A	111.5	C8—C9—C4	120.25 (14)
N1—C2—H2B	111.5	C8—C9—H9A	119.9
C1—C2—H2B	111.5	C4—C9—H9A	119.9
H2A—C2—H2B	109.3	C7—C10—H10A	109.5
N2—C3—N1	116.31 (12)	C7—C10—H10B	109.5
N2—C3—C4	122.68 (12)	H10A—C10—H10B	109.5
N1—C3—C4	120.98 (12)	C7—C10—H10C	109.5
C5—C4—C9	118.72 (12)	H10A—C10—H10C	109.5
C5—C4—C3	119.75 (13)	H10B—C10—H10C	109.5
C9—C4—C3	121.53 (13)		
C3—N2—C1—C2	-5.19 (16)	C9—C4—C5—C6	-1.2 (2)

C3—N1—C2—C1	-11.95 (15)	C3—C4—C5—C6	179.46 (14)
N2—C1—C2—N1	10.31 (15)	C4—C5—C6—C7	0.1 (2)
C1—N2—C3—N1	-2.84 (18)	C5—C6—C7—C8	1.1 (2)
C1—N2—C3—C4	179.35 (13)	C5—C6—C7—C10	-178.05 (14)
C2—N1—C3—N2	10.16 (18)	C6—C7—C8—C9	-1.2 (2)
C2—N1—C3—C4	-171.99 (13)	C10—C7—C8—C9	177.91 (14)
N2—C3—C4—C5	-1.8 (2)	C7—C8—C9—C4	0.2 (2)
N1—C3—C4—C5	-179.56 (14)	C5—C4—C9—C8	1.0 (2)
N2—C3—C4—C9	178.80 (15)	C3—C4—C9—C8	-179.62 (14)
N1—C3—C4—C9	1.1 (2)		

Hydrogen-bond 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—H1N1...N2 ⁱ	0.87 (3)	2.06 (3)	2.9224 (18)	170 (2)
C10—H10B...Cg1 ⁱⁱ	0.96	2.88	3.8110 (16)	163

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Fig. 1

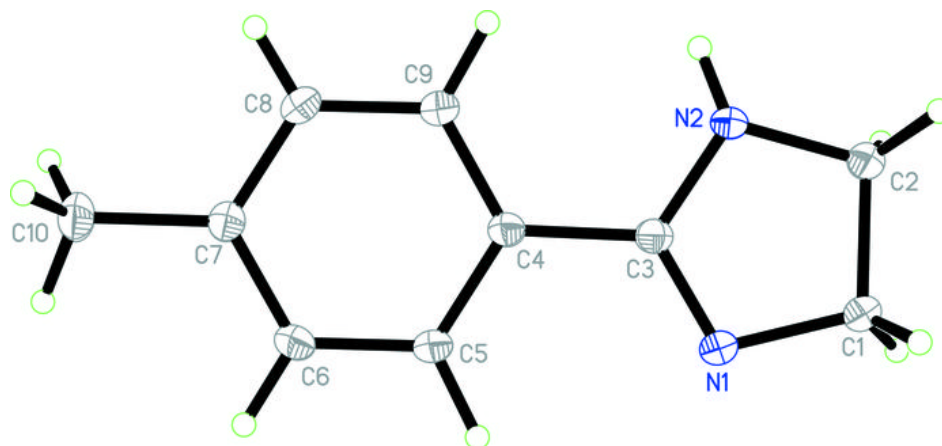


Fig. 2

