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# 4-(4-Methylphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

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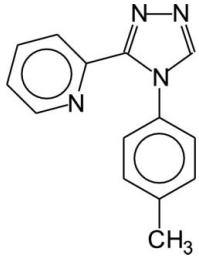
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.053; $wR$ factor = 0.164; data-to-parameter ratio = 15.7.

The crystal structure of the title compound, $C_{14}H_{12}N_4$, is built from two symmetry-independent molecules which are nearly related by translation by the vector **a**/2. The two molecules exhibit almost identical bond distances and angles but they show significantly different conformations. The relative orientations of the pyridyl and benzene rings about the triazole ring are different in the two molecules, and they pack differently in the crystal structure. Weak intermolecular C—H···N, C—H···$\pi$ and $\pi$···$\pi$ interactions stabilize the crystal structure [the distance between the triazole ring centroids is 3.687 (4) Å].

## Related literature

3,4-Diaryl-1,2,4-triazole derivatives have been reported by Mazur *et al.* (2004*a*,*b*), Chinnakali *et al.* (1999) and Rogers *et al.* (1990). For pyridine C—H···N interactions, see also Mootz & Wussow (1981). For related literature, see: Modzelewska (1991/1992).




## Experimental

### *Crystal data*

$C_{14}H_{12}N_4$
$M_r$ = 236.28
Triclinic, $P\overline{1}$
$a$ = 10.730 (2) Å
$b$ = 10.929 (3) Å
$c$ = 11.647 (3) Å
$\alpha$ = 105.21 (3)°
$\beta$ = 99.49 (2)°
$\gamma$ = 108.34 (2)°
$V$ = 1204.5 (6) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.65 mm$^{-1}$
$T$ = 294 (2) K
0.42 × 0.28 × 0.20 mm

### *Data collection*

Kuma KM-4 four-circle diffractometer
Absorption correction: none
5413 measured reflections
5153 independent reflections
1942 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
3 standard reflections every 100 reflections
intensity decay: 0.8%

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.164
$S$ = 0.96
5153 reflections
328 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

The center of the pyridyl ring is denoted as $\pi$.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8a—H8a···N1b | 0.93 | 2.83 | 3.502 (3) | 130 |
| C8a—H8a···N2b | 0.93 | 2.89 | 3.502 (3) | 125 |
| C5a—H5a···N1a$^{i}$ | 0.93 | 2.60 | 3.376 (3) | 141 |
| C11a—H11a···N6a$^{ii}$ | 0.93 | 2.96 | 3.715 (3) | 140 |
| C18a—H18b···N1a$^{iii}$ | 0.96 | 2.87 | 3.432 (4) | 119 |
| C5b—H5b···N1b$^{iv}$ | 0.93 | 2.48 | 3.244 (3) | 140 |
| C14b—H14b···$\pi^{v}$ | 0.93 | 3.05 | 3.951 (4) | 164 |
| C18a—H18a···N2b$^{vi}$ | 0.96 | 2.69 | 3.623 (3) | 164 |
| C11b—H11b···N6a$^{vii}$ | 0.93 | 2.65 | 3.243 (3) | 122 |
| C17b—H17b···N1a$^{iv}$ | 0.93 | 2.68 | 3.505 (4) | 148 |

Symmetry codes: (i) $-x, -y+2, -z+2$; (ii) $-x, -y+1, -z+1$; (iii) $x, y-1, z$; (iv) $-x+1, -y+2, -z+2$; (v) $-x+1, -y+1, -z+1$; (vi) $x-1, y-1, z$; (vii) $x+1, y, z$.

Data collection: *KM-4 Software* (Kuma Diffraction, 1998); cell refinement: *KM-4 Software*; data reduction: *KM-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97* and *enCIFer* (Allen *et al.*, 2004).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2137).

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# supplementary materials

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# 4-(4-Methylphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

**L. Mazur, A. E. Koziol and B. Modzelewska-Banachiewicz**

## Comment

As an extension of our work on the structural characterization of simple 1,2,4-triazole derivatives, we report here the crystal and molecular structure of 4-(4-methylphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole, (I). So far, only four structures of 3,4-diaryl-1,2,4-triazole derivatives have been described in literature [refcodes: WAKBEQ, HAMSUK, GOLYUB, VEXPIX; Mazur *et al.* (2004*a*; 2004*b*), Chinnakali *et al.* (1999) and Rogers *et al.* (1990)].

The crystal of the title compound (Fig. 1) contains two crystallographically independent molecules in the asymmetric unit. Molecules IA and IB are related by apseudo-translation along the *a* axis; the vector being about a/2. Corresponding bond lengths and angles are equal within experimental errors. The central five-membered triazole rings in both molecules have planar geometry. The N1=C5 and N2=C3 bonds display double-bond character, with the bond lengths of 1.282 (4), 1.306 (3) Å for molecule IA and 1.289 (3), 1.315 (3) Å for molecule IB. The N4—C3 and N4—C5 bonds, being in the range 1.353 (3) − 1.367 (3) Å, have an intermediate character. The remaining bond lengths show no unusual values. The only significant difference between the two independent molecules is in dihedral angles between the triazole/pyridyl and triazole/phenyl rings, which are 43.9 (2)°, 44.8 (2)° (molecule IA) and 23.1 (2)°, 60.4 (3)° (molecule IB) (Fig. 2). In a closely related compounds: 4-(4-methylphenyl)-3-(4-pyridyl)-4*H*-1,2,4-triazole (WAKBEQ), and 4-phenyl-3-(4-pyridyl)-4*H*-1,2,4-triazole (HAMSUK), they were 25.2 (3)°, 67.0 (3)° and 46.8 (4)°, 55.9 (3)°, respectively.

Analysis of the intermolecular contacts reveals existence of numerous C—H···N/π and π···π interactions. The most characteristic motifs, observed in this structure, are centrosymmetric dimers created separately by the molecules IA and IB (Figs 3 and 4). Molecules forming these pairs are connected by short quite linear C5a—H5a···N1a and C5b—H5b···N1b hydrogen bonds, with interatomic C···N distances of 3.375 (3) and 3.243 (3) Å (Table 1). The same synthon [with C5···N1 distances of 3.336 (3) and 3.399 (3) Å] was observed in the structure of 3-(4-methoxyphenyl)-4-phenyl-4*H*-1,2,4-triazole (VEXPIX). The triazole N1a atom is also the acceptor in the C17*b*—H17*b*···N1a hydrogen bond. This interaction, accompanied by C11*b*—H11*b*···N6a contact, link adjacent centrosymetric dimers into tetramers. The closest distance between the central five-membered rings in neigbouring dimers indicate the existence of π···π interactions. The distances between the ring centroids of the triazole IA and IB systems are 3.687 (4) Å, with the dihedral angle between their planes of 1.0 (1) °. Other C—H···N and C—H···π hydrogen bonds are also formed and they contribute to the structure stabilization (Table 1).

## Experimental

The title compound was synthesized according to a literature method (Modzelewska, 1991/1992) in reaction of N3-substituted amidrazone with diethylethoxymethylene malonate. Needle-shaped orange single crystals, suitable for X-ray diffraction measurements, were obtained by recrystallization from methanol at room temperature. The melting point determined on a Boëtius microscope was 392 K.

### Refinement

All H atoms were positioned geometrically and constrained, with C—H bond distances of 0.93 and 0.96Å for aromatic and methylene H atom, respectively. The displacement parameters of the H atoms were $U_{iso}$(H) = 1.2 $U_{eq}$(C).

### Figures

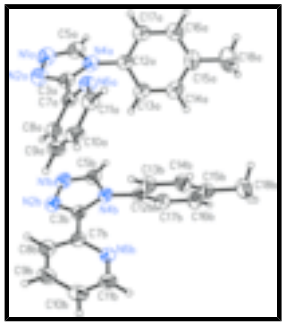

Fig. 1. A view of the two independent molecules of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

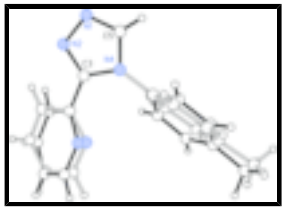

Fig. 2. Fit of the molecules IA (full lines) and IB (open lines).

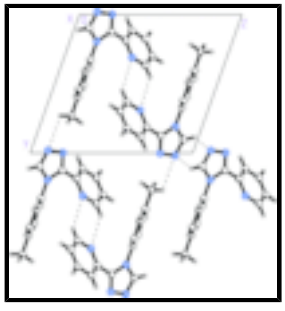

Fig. 3. The packing arrangement of molecules IA, viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

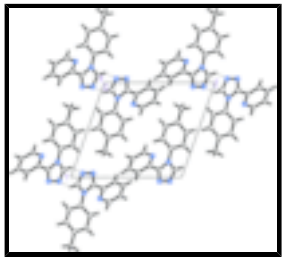

Fig. 4. The packing arrangement of molecules IB, viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

### 4-(4-methylphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

*Crystal data*

| | |
|---|---|
| $C_{14}H_{12}N_4$ | $Z = 4$ |
| $M_r = 236.28$ | $F_{000} = 496$ |

| | |
|---|---|
| Triclinic, $P\bar{1}$ | $D_x$ = 1.303 Mg m$^{-3}$ |
| Hall symbol: -P1 | Cu $K\alpha$ radiation<br>λ = 1.54178 Å |
| $a$ = 10.730 (2) Å | Cell parameters from 40 reflections |
| $b$ = 10.929 (3) Å | θ = 7–21º |
| $c$ = 11.647 (3) Å | μ = 0.65 mm$^{-1}$ |
| α = 105.21 (3)º | $T$ = 294 (2) K |
| β = 99.49 (2)º | Needle, orange |
| γ = 108.34 (2)º | 0.42 × 0.28 × 0.20 mm |
| $V$ = 1204.5 (6) Å$^3$ | |

*Data collection*

| | |
|---|---|
| KM4 four-circle diffractometer | $R_{int}$ = 0.039 |
| Radiation source: fine-focus sealed tube | $\theta_{max}$ = 80.3º |
| Monochromator: graphite | $\theta_{min}$ = 4.5º |
| $T$ = 293(2) K | $h$ = −13→13 |
| ω–2θ scans | $k$ = −12→12 |
| Absorption correction: none | $l$ = 0→14 |
| 5413 measured reflections | 3 standard reflections |
| 5153 independent reflections | every 100 reflections |
| 1942 reflections with $I > 2\sigma(I)$ | intensity decay: 0.8% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.053 | $w = 1/[\sigma^2(F_o^2) + (0.0867P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.164 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 0.96 | $\Delta\rho_{max}$ = 0.24 e Å$^{-3}$ |
| 5153 reflections | $\Delta\rho_{min}$ = −0.20 e Å$^{-3}$ |
| 328 parameters | Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0050 (7) |
| Secondary atom site location: difference Fourier map | |

*Special details*

**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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1A | 0.1149 (3) | 1.0190 (3) | 0.8957 (2) | 0.0818 (7) |
| N2A | 0.1763 (3) | 1.0022 (2) | 0.7996 (2) | 0.0752 (7) |
| C3A | 0.1689 (3) | 0.8757 (3) | 0.7654 (2) | 0.0593 (7) |
| N4A | 0.1048 (2) | 0.8077 (2) | 0.83452 (18) | 0.0605 (6) |
| C5A | 0.0748 (3) | 0.9036 (3) | 0.9134 (2) | 0.0719 (8) |
| H5A | 0.0304 | 0.8873 | 0.9732 | 0.086* |
| N6A | 0.1279 (2) | 0.6903 (2) | 0.58261 (18) | 0.0600 (6) |
| C7A | 0.2148 (3) | 0.8145 (3) | 0.6605 (2) | 0.0555 (6) |
| C8A | 0.3372 (3) | 0.8835 (3) | 0.6424 (3) | 0.0646 (7) |
| H8A | 0.3949 | 0.9693 | 0.6978 | 0.078* |
| C9A | 0.3721 (3) | 0.8224 (3) | 0.5405 (3) | 0.0731 (8) |
| H9A | 0.4547 | 0.8663 | 0.5263 | 0.088* |
| C10A | 0.2861 (3) | 0.6981 (3) | 0.4608 (3) | 0.0701 (8) |
| H10A | 0.3083 | 0.6562 | 0.3910 | 0.084* |
| C11A | 0.1649 (3) | 0.6344 (3) | 0.4844 (2) | 0.0649 (7) |
| H11A | 0.1065 | 0.5487 | 0.4293 | 0.078* |
| C12A | 0.0823 (3) | 0.6717 (3) | 0.8335 (2) | 0.0562 (6) |
| C13A | 0.1852 (3) | 0.6218 (3) | 0.8270 (2) | 0.0659 (7) |
| H13A | 0.2702 | 0.6775 | 0.8253 | 0.079* |
| C14A | 0.1616 (3) | 0.4907 (3) | 0.8231 (2) | 0.0726 (8) |
| H14A | 0.2303 | 0.4567 | 0.8157 | 0.087* |
| C15A | 0.0382 (4) | 0.4071 (3) | 0.8298 (2) | 0.0708 (8) |
| C16A | −0.0622 (3) | 0.4601 (3) | 0.8402 (2) | 0.0724 (8) |
| H16A | −0.1450 | 0.4065 | 0.8477 | 0.087* |
| C17A | −0.0419 (3) | 0.5902 (3) | 0.8395 (2) | 0.0653 (7) |
| H17A | −0.1117 | 0.6231 | 0.8432 | 0.078* |
| C18A | 0.0169 (5) | 0.2674 (4) | 0.8271 (3) | 0.1151 (14) |
| H18A | −0.0729 | 0.2244 | 0.8347 | 0.138* |
| H18B | 0.0835 | 0.2696 | 0.8945 | 0.138* |
| H18C | 0.0260 | 0.2164 | 0.7503 | 0.138* |
| N1B | 0.6153 (3) | 1.0428 (3) | 0.9064 (2) | 0.0752 (7) |
| N2B | 0.6802 (2) | 1.0421 (2) | 0.8128 (2) | 0.0709 (7) |
| C3B | 0.6823 (3) | 0.9191 (3) | 0.7699 (2) | 0.0573 (6) |
| N4B | 0.6204 (2) | 0.8386 (2) | 0.83221 (19) | 0.0574 (5) |
| C5B | 0.5823 (3) | 0.9222 (3) | 0.9150 (3) | 0.0664 (7) |
| H5B | 0.5375 | 0.8956 | 0.9715 | 0.080* |
| N6B | 0.7863 (2) | 0.7749 (2) | 0.6687 (2) | 0.0620 (6) |
| C7B | 0.7465 (3) | 0.8793 (3) | 0.6717 (2) | 0.0571 (6) |
| C8B | 0.7638 (3) | 0.9491 (3) | 0.5891 (3) | 0.0719 (8) |
| H8B | 0.7340 | 1.0211 | 0.5940 | 0.086* |

| | | | | |
|---|---|---|---|---|
| C9B | 0.8257 (3) | 0.9106 (3) | 0.4994 (3) | 0.0764 (8) |
| H9B | 0.8397 | 0.9567 | 0.4431 | 0.092* |
| C10B | 0.8663 (3) | 0.8033 (3) | 0.4946 (3) | 0.0754 (8) |
| H10B | 0.9078 | 0.7742 | 0.4344 | 0.090* |
| C11B | 0.8448 (3) | 0.7394 (3) | 0.5798 (3) | 0.0700 (8) |
| H11B | 0.8727 | 0.6663 | 0.5755 | 0.084* |
| C12B | 0.5911 (2) | 0.6965 (3) | 0.8157 (2) | 0.0524 (6) |
| C13B | 0.5098 (3) | 0.5971 (3) | 0.7054 (2) | 0.0666 (7) |
| H13B | 0.4753 | 0.6208 | 0.6395 | 0.080* |
| C14B | 0.4803 (3) | 0.4615 (3) | 0.6944 (3) | 0.0705 (8) |
| H14B | 0.4264 | 0.3943 | 0.6195 | 0.085* |
| C15B | 0.5278 (3) | 0.4222 (3) | 0.7906 (3) | 0.0644 (7) |
| C16B | 0.6077 (3) | 0.5243 (3) | 0.8987 (3) | 0.0727 (8) |
| H16B | 0.6409 | 0.5007 | 0.9652 | 0.087* |
| C17B | 0.6408 (3) | 0.6611 (3) | 0.9130 (2) | 0.0666 (7) |
| H17B | 0.6960 | 0.7282 | 0.9875 | 0.080* |
| C18B | 0.4940 (4) | 0.2749 (3) | 0.7794 (3) | 0.0997 (11) |
| H18D | 0.5056 | 0.2265 | 0.7028 | 0.120* |
| H18E | 0.4012 | 0.2350 | 0.7812 | 0.120* |
| H18F | 0.5536 | 0.2688 | 0.8470 | 0.120* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1A | 0.097 (2) | 0.0727 (17) | 0.0715 (16) | 0.0414 (16) | 0.0257 (14) | 0.0042 (13) |
| N2A | 0.0837 (18) | 0.0649 (16) | 0.0712 (15) | 0.0312 (13) | 0.0238 (13) | 0.0081 (12) |
| C3A | 0.0594 (17) | 0.0569 (16) | 0.0549 (15) | 0.0247 (13) | 0.0127 (13) | 0.0064 (12) |
| N4A | 0.0658 (15) | 0.0629 (14) | 0.0499 (11) | 0.0308 (12) | 0.0157 (11) | 0.0063 (10) |
| C5A | 0.082 (2) | 0.077 (2) | 0.0556 (15) | 0.0389 (17) | 0.0246 (15) | 0.0054 (14) |
| N6A | 0.0597 (14) | 0.0637 (14) | 0.0515 (12) | 0.0230 (11) | 0.0193 (11) | 0.0090 (10) |
| C7A | 0.0571 (16) | 0.0565 (16) | 0.0530 (14) | 0.0250 (13) | 0.0143 (12) | 0.0143 (12) |
| C8A | 0.0555 (17) | 0.0635 (17) | 0.0701 (17) | 0.0195 (14) | 0.0116 (14) | 0.0216 (14) |
| C9A | 0.0603 (18) | 0.092 (2) | 0.0764 (19) | 0.0302 (18) | 0.0286 (16) | 0.0359 (18) |
| C10A | 0.0701 (19) | 0.095 (2) | 0.0597 (16) | 0.0442 (18) | 0.0280 (15) | 0.0268 (16) |
| C11A | 0.077 (2) | 0.0669 (17) | 0.0510 (14) | 0.0335 (15) | 0.0223 (14) | 0.0092 (13) |
| C12A | 0.0604 (16) | 0.0653 (17) | 0.0412 (12) | 0.0273 (14) | 0.0149 (12) | 0.0101 (11) |
| C13A | 0.0654 (18) | 0.075 (2) | 0.0611 (16) | 0.0336 (16) | 0.0160 (14) | 0.0209 (14) |
| C14A | 0.081 (2) | 0.086 (2) | 0.0563 (16) | 0.0413 (18) | 0.0171 (15) | 0.0220 (15) |
| C15A | 0.101 (3) | 0.0659 (19) | 0.0439 (14) | 0.0323 (18) | 0.0156 (15) | 0.0168 (12) |
| C16A | 0.077 (2) | 0.084 (2) | 0.0523 (15) | 0.0225 (17) | 0.0209 (14) | 0.0232 (15) |
| C17A | 0.0659 (18) | 0.082 (2) | 0.0483 (14) | 0.0320 (16) | 0.0189 (13) | 0.0146 (13) |
| C18A | 0.154 (4) | 0.092 (3) | 0.092 (3) | 0.035 (3) | 0.031 (3) | 0.033 (2) |
| N1B | 0.0827 (18) | 0.0697 (17) | 0.0814 (16) | 0.0419 (14) | 0.0315 (14) | 0.0164 (13) |
| N2B | 0.0688 (16) | 0.0634 (15) | 0.0861 (17) | 0.0317 (13) | 0.0259 (14) | 0.0225 (13) |
| C3B | 0.0567 (16) | 0.0567 (16) | 0.0619 (15) | 0.0266 (13) | 0.0178 (13) | 0.0179 (12) |
| N4B | 0.0634 (14) | 0.0603 (14) | 0.0557 (12) | 0.0322 (11) | 0.0214 (10) | 0.0166 (10) |
| C5B | 0.0747 (19) | 0.0677 (19) | 0.0667 (16) | 0.0385 (16) | 0.0294 (15) | 0.0174 (14) |
| N6B | 0.0606 (13) | 0.0645 (14) | 0.0703 (14) | 0.0307 (12) | 0.0259 (11) | 0.0235 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7B | 0.0528 (15) | 0.0573 (16) | 0.0599 (15) | 0.0218 (13) | 0.0139 (12) | 0.0172 (12) |
| C8B | 0.069 (2) | 0.080 (2) | 0.0763 (19) | 0.0324 (16) | 0.0207 (16) | 0.0344 (16) |
| C9B | 0.0662 (19) | 0.097 (2) | 0.0742 (19) | 0.0267 (18) | 0.0262 (16) | 0.0413 (18) |
| C10B | 0.0623 (19) | 0.096 (2) | 0.0659 (18) | 0.0261 (17) | 0.0258 (15) | 0.0225 (16) |
| C11B | 0.0616 (18) | 0.0711 (19) | 0.083 (2) | 0.0304 (15) | 0.0315 (16) | 0.0209 (15) |
| C12B | 0.0547 (15) | 0.0554 (15) | 0.0531 (14) | 0.0263 (13) | 0.0196 (12) | 0.0176 (12) |
| C13B | 0.0665 (18) | 0.0672 (18) | 0.0590 (16) | 0.0230 (15) | 0.0070 (14) | 0.0189 (14) |
| C14B | 0.068 (2) | 0.0587 (18) | 0.0703 (18) | 0.0147 (15) | 0.0133 (15) | 0.0133 (14) |
| C15B | 0.0644 (19) | 0.0634 (17) | 0.0708 (17) | 0.0250 (15) | 0.0269 (15) | 0.0247 (14) |
| C16B | 0.087 (2) | 0.075 (2) | 0.0647 (18) | 0.0337 (17) | 0.0207 (16) | 0.0332 (15) |
| C17B | 0.075 (2) | 0.0691 (18) | 0.0546 (15) | 0.0292 (15) | 0.0163 (14) | 0.0175 (13) |
| C18B | 0.108 (3) | 0.071 (2) | 0.128 (3) | 0.030 (2) | 0.046 (2) | 0.042 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1A—C5A | 1.282 (4) | N1B—C5B | 1.289 (3) |
| N1A—N2A | 1.390 (3) | N1B—N2B | 1.386 (3) |
| N2A—C3A | 1.306 (3) | N2B—C3B | 1.315 (3) |
| C3A—N4A | 1.360 (3) | C3B—N4B | 1.367 (3) |
| C3A—C7A | 1.470 (3) | C3B—C7B | 1.468 (3) |
| N4A—C5A | 1.360 (3) | N4B—C5B | 1.353 (3) |
| N4A—C12A | 1.425 (3) | N4B—C12B | 1.437 (3) |
| C5A—H5A | 0.9300 | C5B—H5B | 0.9300 |
| N6A—C11A | 1.332 (3) | N6B—C11B | 1.331 (3) |
| N6A—C7A | 1.347 (3) | N6B—C7B | 1.333 (3) |
| C7A—C8A | 1.374 (4) | C7B—C8B | 1.378 (4) |
| C8A—C9A | 1.373 (4) | C8B—C9B | 1.372 (4) |
| C8A—H8A | 0.9300 | C8B—H8B | 0.9300 |
| C9A—C10A | 1.351 (4) | C9B—C10B | 1.365 (4) |
| C9A—H9A | 0.9300 | C9B—H9B | 0.9300 |
| C10A—C11A | 1.378 (4) | C10B—C11B | 1.365 (4) |
| C10A—H10A | 0.9300 | C10B—H10B | 0.9300 |
| C11A—H11A | 0.9300 | C11B—H11B | 0.9300 |
| C12A—C17A | 1.375 (4) | C12B—C17B | 1.372 (3) |
| C12A—C13A | 1.381 (3) | C12B—C13B | 1.376 (3) |
| C13A—C14A | 1.361 (4) | C13B—C14B | 1.380 (4) |
| C13A—H13A | 0.9300 | C13B—H13B | 0.9300 |
| C14A—C15A | 1.381 (4) | C14B—C15B | 1.379 (4) |
| C14A—H14A | 0.9300 | C14B—H14B | 0.9300 |
| C15A—C16A | 1.381 (4) | C15B—C16B | 1.368 (4) |
| C15A—C18A | 1.462 (4) | C15B—C18B | 1.499 (4) |
| C16A—C17A | 1.372 (4) | C16B—C17B | 1.379 (4) |
| C16A—H16A | 0.9300 | C16B—H16B | 0.9300 |
| C17A—H17A | 0.9300 | C17B—H17B | 0.9300 |
| C18A—H18A | 0.9600 | C18B—H18D | 0.9600 |
| C18A—H18B | 0.9600 | C18B—H18E | 0.9600 |
| C18A—H18C | 0.9600 | C18B—H18F | 0.9600 |
| C5A—N1A—N2A | 106.6 (2) | C5B—N1B—N2B | 106.5 (2) |
| C3A—N2A—N1A | 107.1 (2) | C3B—N2B—N1B | 107.3 (2) |

| | | | |
|---|---|---|---|
| N2A—C3A—N4A | 110.6 (2) | N2B—C3B—N4B | 109.9 (2) |
| N2A—C3A—C7A | 123.9 (3) | N2B—C3B—C7B | 123.6 (2) |
| N4A—C3A—C7A | 125.3 (2) | N4B—C3B—C7B | 126.5 (2) |
| C3A—N4A—C5A | 103.7 (2) | C5B—N4B—C3B | 104.1 (2) |
| C3A—N4A—C12A | 129.2 (2) | C5B—N4B—C12B | 124.7 (2) |
| C5A—N4A—C12A | 126.9 (2) | C3B—N4B—C12B | 131.1 (2) |
| N1A—C5A—N4A | 112.1 (3) | N1B—C5B—N4B | 112.2 (3) |
| N1A—C5A—H5A | 123.9 | N1B—C5B—H5B | 123.9 |
| N4A—C5A—H5A | 123.9 | N4B—C5B—H5B | 123.9 |
| C11A—N6A—C7A | 117.1 (2) | C11B—N6B—C7B | 116.4 (2) |
| N6A—C7A—C8A | 123.0 (2) | N6B—C7B—C8B | 123.2 (2) |
| N6A—C7A—C3A | 115.8 (2) | N6B—C7B—C3B | 116.6 (2) |
| C8A—C7A—C3A | 121.2 (2) | C8B—C7B—C3B | 120.2 (2) |
| C9A—C8A—C7A | 118.3 (3) | C9B—C8B—C7B | 118.8 (3) |
| C9A—C8A—H8A | 120.9 | C9B—C8B—H8B | 120.6 |
| C7A—C8A—H8A | 120.9 | C7B—C8B—H8B | 120.6 |
| C10A—C9A—C8A | 119.7 (3) | C10B—C9B—C8B | 118.7 (3) |
| C10A—C9A—H9A | 120.1 | C10B—C9B—H9B | 120.7 |
| C8A—C9A—H9A | 120.1 | C8B—C9B—H9B | 120.7 |
| C9A—C10A—C11A | 119.1 (3) | C11B—C10B—C9B | 118.6 (3) |
| C9A—C10A—H10A | 120.5 | C11B—C10B—H10B | 120.7 |
| C11A—C10A—H10A | 120.5 | C9B—C10B—H10B | 120.7 |
| N6A—C11A—C10A | 122.9 (3) | N6B—C11B—C10B | 124.3 (3) |
| N6A—C11A—H11A | 118.6 | N6B—C11B—H11B | 117.9 |
| C10A—C11A—H11A | 118.6 | C10B—C11B—H11B | 117.9 |
| C17A—C12A—C13A | 119.9 (3) | C17B—C12B—C13B | 120.4 (3) |
| C17A—C12A—N4A | 120.0 (3) | C17B—C12B—N4B | 119.1 (2) |
| C13A—C12A—N4A | 120.1 (3) | C13B—C12B—N4B | 120.5 (2) |
| C14A—C13A—C12A | 119.7 (3) | C12B—C13B—C14B | 118.9 (3) |
| C14A—C13A—H13A | 120.2 | C12B—C13B—H13B | 120.6 |
| C12A—C13A—H13A | 120.2 | C14B—C13B—H13B | 120.6 |
| C13A—C14A—C15A | 121.5 (3) | C15B—C14B—C13B | 122.3 (3) |
| C13A—C14A—H14A | 119.2 | C15B—C14B—H14B | 118.9 |
| C15A—C14A—H14A | 119.2 | C13B—C14B—H14B | 118.9 |
| C14A—C15A—C16A | 118.0 (3) | C16B—C15B—C14B | 117.0 (3) |
| C14A—C15A—C18A | 120.2 (3) | C16B—C15B—C18B | 120.7 (3) |
| C16A—C15A—C18A | 121.8 (3) | C14B—C15B—C18B | 122.3 (3) |
| C17A—C16A—C15A | 121.2 (3) | C15B—C16B—C17B | 122.5 (3) |
| C17A—C16A—H16A | 119.4 | C15B—C16B—H16B | 118.7 |
| C15A—C16A—H16A | 119.4 | C17B—C16B—H16B | 118.7 |
| C16A—C17A—C12A | 119.6 (3) | C12B—C17B—C16B | 119.0 (3) |
| C16A—C17A—H17A | 120.2 | C12B—C17B—H17B | 120.5 |
| C12A—C17A—H17A | 120.2 | C16B—C17B—H17B | 120.5 |
| C15A—C18A—H18A | 109.5 | C15B—C18B—H18D | 109.5 |
| C15A—C18A—H18B | 109.5 | C15B—C18B—H18E | 109.5 |
| H18A—C18A—H18B | 109.5 | H18D—C18B—H18E | 109.5 |
| C15A—C18A—H18C | 109.5 | C15B—C18B—H18F | 109.5 |
| H18A—C18A—H18C | 109.5 | H18D—C18B—H18F | 109.5 |
| H18B—C18A—H18C | 109.5 | H18E—C18B—H18F | 109.5 |

| | | | |
|---|---|---|---|
| C5A—N1A—N2A—C3A | 0.0 (3) | C5B—N1B—N2B—C3B | 0.1 (3) |
| N1A—N2A—C3A—N4A | 0.2 (3) | N1B—N2B—C3B—N4B | 0.2 (3) |
| N1A—N2A—C3A—C7A | 175.9 (2) | N1B—N2B—C3B—C7B | −178.2 (2) |
| N2A—C3A—N4A—C5A | −0.3 (3) | N2B—C3B—N4B—C5B | −0.3 (3) |
| C7A—C3A—N4A—C5A | −176.0 (3) | C7B—C3B—N4B—C5B | 178.0 (3) |
| N2A—C3A—N4A—C12A | −175.8 (3) | N2B—C3B—N4B—C12B | 176.4 (2) |
| C7A—C3A—N4A—C12A | 8.5 (4) | C7B—C3B—N4B—C12B | −5.3 (4) |
| N2A—N1A—C5A—N4A | −0.2 (3) | N2B—N1B—C5B—N4B | −0.3 (3) |
| C3A—N4A—C5A—N1A | 0.3 (3) | C3B—N4B—C5B—N1B | 0.4 (3) |
| C12A—N4A—C5A—N1A | 176.0 (3) | C12B—N4B—C5B—N1B | −176.6 (2) |
| C11A—N6A—C7A—C8A | −0.1 (4) | C11B—N6B—C7B—C8B | −0.2 (4) |
| C11A—N6A—C7A—C3A | 177.8 (2) | C11B—N6B—C7B—C3B | −179.8 (3) |
| N2A—C3A—C7A—N6A | −133.3 (3) | N2B—C3B—C7B—N6B | 155.7 (3) |
| N4A—C3A—C7A—N6A | 41.9 (4) | N4B—C3B—C7B—N6B | −22.4 (4) |
| N2A—C3A—C7A—C8A | 44.7 (4) | N2B—C3B—C7B—C8B | −23.9 (4) |
| N4A—C3A—C7A—C8A | −140.2 (3) | N4B—C3B—C7B—C8B | 158.1 (3) |
| N6A—C7A—C8A—C9A | −0.2 (4) | N6B—C7B—C8B—C9B | −0.4 (4) |
| C3A—C7A—C8A—C9A | −178.0 (2) | C3B—C7B—C8B—C9B | 179.1 (3) |
| C7A—C8A—C9A—C10A | 0.5 (4) | C7B—C8B—C9B—C10B | 0.8 (5) |
| C8A—C9A—C10A—C11A | −0.6 (5) | C8B—C9B—C10B—C11B | −0.6 (5) |
| C7A—N6A—C11A—C10A | 0.0 (4) | C7B—N6B—C11B—C10B | 0.5 (4) |
| C9A—C10A—C11A—N6A | 0.3 (5) | C9B—C10B—C11B—N6B | −0.1 (5) |
| C3A—N4A—C12A—C17A | −137.7 (3) | C5B—N4B—C12B—C17B | −60.9 (3) |
| C5A—N4A—C12A—C17A | 47.7 (4) | C3B—N4B—C12B—C17B | 123.0 (3) |
| C3A—N4A—C12A—C13A | 42.7 (4) | C5B—N4B—C12B—C13B | 116.6 (3) |
| C5A—N4A—C12A—C13A | −132.0 (3) | C3B—N4B—C12B—C13B | −59.6 (4) |
| C17A—C12A—C13A—C14A | 1.9 (4) | C17B—C12B—C13B—C14B | −0.5 (4) |
| N4A—C12A—C13A—C14A | −178.4 (2) | N4B—C12B—C13B—C14B | −177.9 (2) |
| C12A—C13A—C14A—C15A | −2.3 (4) | C12B—C13B—C14B—C15B | 1.0 (4) |
| C13A—C14A—C15A—C16A | 0.3 (4) | C13B—C14B—C15B—C16B | −0.6 (4) |
| C13A—C14A—C15A—C18A | −179.1 (3) | C13B—C14B—C15B—C18B | 179.0 (3) |
| C14A—C15A—C16A—C17A | 2.2 (4) | C14B—C15B—C16B—C17B | −0.2 (4) |
| C18A—C15A—C16A—C17A | −178.4 (3) | C18B—C15B—C16B—C17B | −179.8 (3) |
| C15A—C16A—C17A—C12A | −2.6 (4) | C13B—C12B—C17B—C16B | −0.2 (4) |
| C13A—C12A—C17A—C16A | 0.6 (4) | N4B—C12B—C17B—C16B | 177.2 (2) |
| N4A—C12A—C17A—C16A | −179.1 (2) | C15B—C16B—C17B—C12B | 0.6 (5) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8a—H8a···N1b | 0.93 | 2.83 | 3.502 (3) | 130 |
| C8a—H8a···N2b | 0.93 | 2.89 | 3.502 (3) | 125 |
| C5a—H5a···N1a$^{i}$ | 0.93 | 2.60 | 3.376 (3) | 141 |
| C11a—H11a···N6a$^{ii}$ | 0.93 | 2.96 | 3.715 (3) | 140 |
| C18a—H18b···N1a$^{iii}$ | 0.96 | 2.87 | 3.432 (4) | 119 |
| C5b—H5b···N1b$^{iv}$ | 0.93 | 2.48 | 3.244 (3) | 140 |
| C14b—H14b···$\pi^{v}$ | 0.93 | 3.05 | 3.951 (4) | 164 |
| C18a—H18a···N2b$^{vi}$ | 0.96 | 2.69 | 3.623 (3) | 164 |

| | | | | |
|---|---|---|---|---|
| C11b—H11b···N6a$^{vii}$ | 0.93 | 2.65 | 3.243 (3) | 122 |
| C17b—H17b···N1a$^{iv}$ | 0.93 | 2.68 | 3.505 (4) | 148 |

Symmetry codes: (i) −*x*, −*y*+2, −*z*+2; (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) −*x*+1, −*y*+2, −*z*+2; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*−1, *y*−1, *z*; (vii) *x*+1, *y*, *z*.

**Fig. 1**

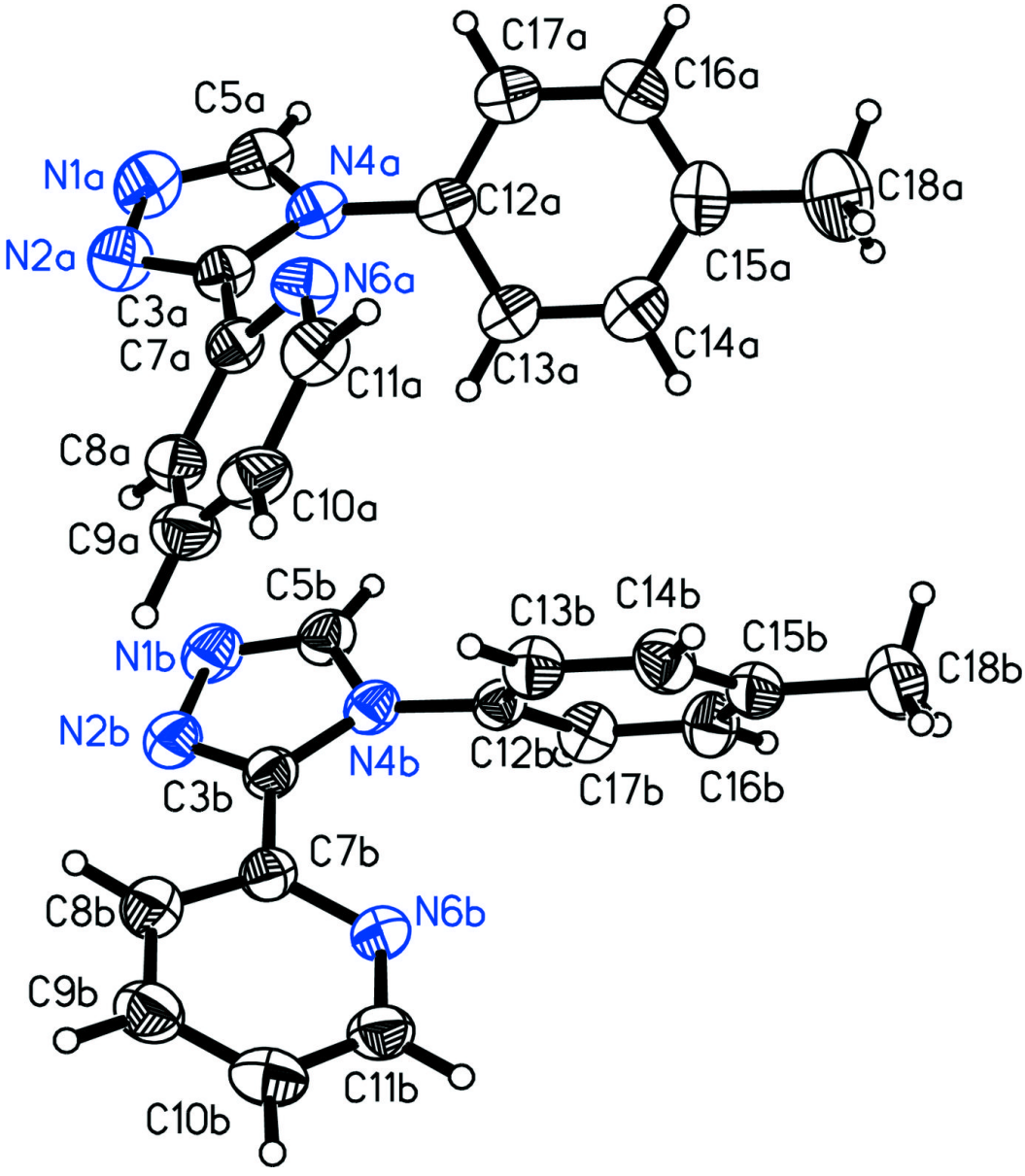
C17a
C16a
C5a
N1a
N4a
C12a
C18a
N2a
C15a
N6a
C3a
C7a
C14a
C13a
C11a
C8a
C10a
C9a
C5b
C13b
C14b
C15b
C18b
N1b
N2b
N4b
C12b
C17b
C16b
C3b
C7b
C8b
N6b
C9b
C11b
C10b

**Fig. 2**

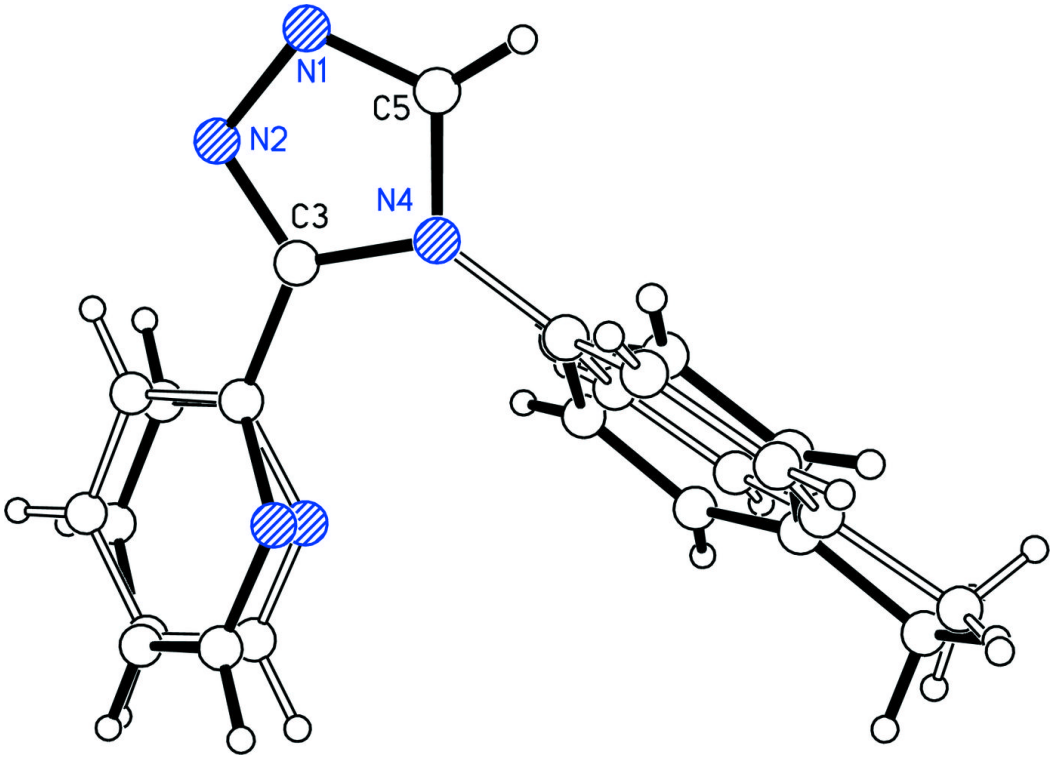

**Fig. 3**

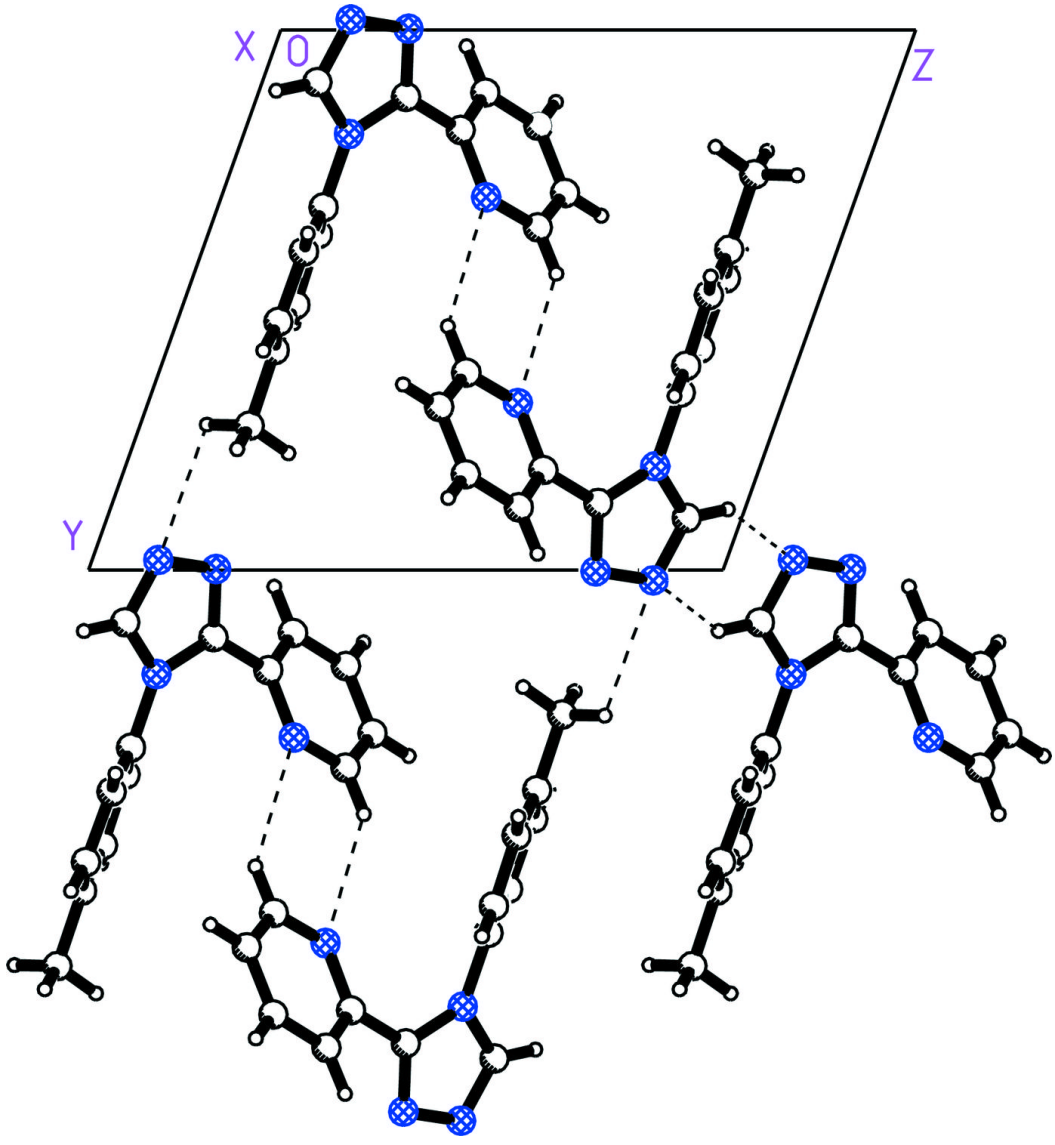

Fig. 4