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# 2-{4-[5-(3-Pyridyl)-2*H*-tetrazol-2-ylmethyl]phenyl}benzonitrile

**Wei Dai and Da-Wei Fu***

Ordered Matter Science Research Center, College of Chemistry and Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: fudavid88@yahoo.com.cn

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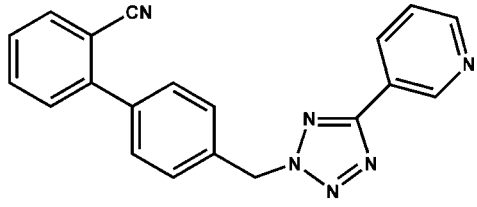
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.079; $wR$ factor = 0.239; data-to-parameter ratio = 17.1.

In the title compound, $C_{20}H_{14}N_6$, there are two molecules with similar conformations in the asymmetric unit. The pyridine and tetrazole rings are nearly coplanar; they are twisted from each other by dihedral angles of only 8.7 (2) and 7.4 (2)°. The nearer benzene ring makes dihedral angles of 69.9 (2) and 88.5 (2)° with the tetrazole ring in the two molecules.

## Related literature

For the use of tetrazole derivatives in coordination chemistry, see: Arp *et al.* (2000); Hu *et al.* (2007); Wang *et al.* (2005); Xiong *et al.* (2002).




## Experimental

### *Crystal data*

$C_{20}H_{14}N_6$ $M_r$ = 338.37
Triclinic, $P\overline{1}$
$a$ = 10.2096 (9) Å
$b$ = 13.3071 (16) Å
$c$ = 13.709 (2) Å
$\alpha$ = 77.24 (2)°
$\beta$ = 69.08 (2)°
$\gamma$ = 83.52 (3)°
$V$ = 1695.6 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 (2) K
0.4 × 0.35 × 0.35 mm

### *Data collection*

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.958, $T_{max}$ = 0.969
18012 measured reflections
8011 independent reflections
3834 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.239
$S$ = 1.02
8011 reflections
469 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2354).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o1444 [ **doi:10.1107/S1600536808017959** ]

# 2-{4-[5-(3-Pyridyl)-2*H*-tetrazol-2-ylmethyl]phenyl}benzonitrile

**W. Dai and D.-W. Fu**

## Comment

In the past five years, our work have been focused on the chemistry of tetrazole derivatives because of their multiple coordination modes as ligands to metal ions and for the construction of novel metal-organic frameworks (Wang, *et al.* 2005; Xiong, *et al.* 2002). We report here the crystal structure of the title compound, 4-(4-((5-(pyridin-3-yl)-2*H*-tetrazol-2-yl)methyl)phenyl)benzonitrile.

The title compound contains two molecules with similar conformation in the asymmetrric unit. Each molecule is built up by four different rings (Fig.1). The pyridine and tetrazole rings are nearly coplanar and are only twisted from each other by a dihedral angle of 8.7 (2)° [7.4 (2)° for the second molecule]. The benzene ring makes a dihedral angle of 69.9 (2)° [88.5 (2)°] with the tetrazole ring owing to the methylene bridge which forces the two rings to be twisted from each other. The benzonitrile and the phenyl ring attached to it are twisted and make a dihedral angle of 46.5 (1)° [48.1 (2)°]. The C1—N1 and C21—N7 bond length of 1.153Å and 1.124Å conforms to the value for a C≡N bond. The bond distances and bond angles of the tetrazole rings are in the usual ranges (Wang *et al.*, 2005; Arp *et al.*, 2000; Hu *et al.*, 2007).

## Experimental

4-(4-((5-(Pyridin-3-yl)-2*H*-tetrazol-2-yl)methyl) phenyl)benzonitrile (3 mmol) was dissolved in ethanol (20 ml) and evaporated in the air affording colorless block crystals of this compound suitable for X-ray analysis were obtained.

## Refinement

All H atoms were fixed geometrically and treated as riding with C–H = 0.93Å (methine), 0.97 Å(methylene), with $U_{iso}$(H) =1.2Ueq(C).

## Figures

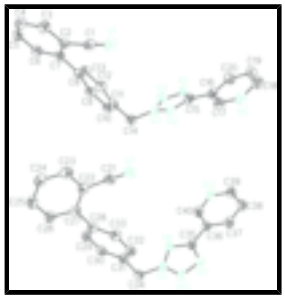


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level. H atoms were omitted for clarity.

**2-{4-[5-(3-pyridyl)-2*H*-tetrazol-2-ylmethyl]phenyl}benzonitrile**

*Crystal data*

| | |
|---|---|
| $C_{20}H_{14}N_6$ | $Z = 4$ |
| $M_r = 338.37$ | $F_{000} = 704$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.325$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 10.2096$ (9) Å | Cell parameters from 3792 reflections |
| $b = 13.3071$ (16) Å | $\theta = 3.4$–$27.5$º |
| $c = 13.709$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $\alpha = 77.24$ (2)º | $T = 293$ (2) K |
| $\beta = 69.08$ (2)º | Block, colourless |
| $\gamma = 83.52$ (3)º | 0.4 × 0.35 × 0.35 mm |
| $V = 1695.6$ (4) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Rigaku Mercury2 (2x2 bin mode) diffractometer | 8011 independent reflections |
| Radiation source: fine-focus sealed tube | 3834 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.060$ |
| Detector resolution: 13.6612 pixels mm$^{-1}$ | $\theta_{max} = 27.9$º |
| $T = 293$(2) K | $\theta_{min} = 2.5$º |
| ω scans | $h = -13 \rightarrow 13$ |
| Absorption correction: multi-scan (CrystalClear; Rigaku, 2005) | $k = -17 \rightarrow 17$ |
| $T_{min} = 0.958$, $T_{max} = 0.969$ | $l = -17 \rightarrow 18$ |
| 18012 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.079$ | H-atom parameters constrained |
| $wR(F^2) = 0.239$ | $w = 1/[\sigma^2(F_o^2) + (0.1033P)^2 + 0.086P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} = 0.033$ |
| 8011 reflections | $\Delta\rho_{max} = 0.22$ e Å$^{-3}$ |
| 469 parameters | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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.

**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 ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.2892 (3) | 0.4722 (3) | −0.0251 (3) | 0.0493 (8) |
| C2 | 0.1973 (3) | 0.5487 (2) | −0.0616 (3) | 0.0468 (8) |
| C3 | 0.1710 (4) | 0.5407 (3) | −0.1523 (3) | 0.0607 (9) |
| H3 | 0.2188 | 0.4901 | −0.1906 | 0.073* |
| C4 | 0.0765 (4) | 0.6058 (3) | −0.1859 (3) | 0.0666 (10) |
| H4 | 0.0610 | 0.6006 | −0.2474 | 0.080* |
| C5 | 0.0034 (4) | 0.6799 (3) | −0.1279 (3) | 0.0651 (10) |
| H5 | −0.0644 | 0.7228 | −0.1487 | 0.078* |
| C6 | 0.0313 (4) | 0.6901 (3) | −0.0390 (3) | 0.0573 (9) |
| H6 | −0.0172 | 0.7410 | −0.0015 | 0.069* |
| C7 | 0.1297 (3) | 0.6266 (2) | −0.0042 (3) | 0.0452 (8) |
| C8 | 0.1637 (3) | 0.6414 (2) | 0.0893 (3) | 0.0454 (8) |
| C9 | 0.3033 (3) | 0.6420 (2) | 0.0825 (3) | 0.0457 (8) |
| H9 | 0.3748 | 0.6343 | 0.0193 | 0.055* |
| C10 | 0.3369 (3) | 0.6542 (2) | 0.1689 (3) | 0.0487 (8) |
| H10 | 0.4306 | 0.6538 | 0.1627 | 0.058* |
| C11 | 0.2337 (3) | 0.6667 (2) | 0.2634 (3) | 0.0461 (8) |
| C12 | 0.0941 (4) | 0.6678 (3) | 0.2696 (3) | 0.0547 (9) |
| H12 | 0.0227 | 0.6776 | 0.3321 | 0.066* |
| C13 | 0.0601 (3) | 0.6544 (3) | 0.1838 (3) | 0.0522 (8) |
| H13 | −0.0337 | 0.6542 | 0.1901 | 0.063* |
| C14 | 0.2711 (4) | 0.6775 (3) | 0.3571 (3) | 0.0555 (9) |
| H14A | 0.3618 | 0.7085 | 0.3311 | 0.067* |
| H14B | 0.2025 | 0.7239 | 0.3963 | 0.067* |
| C15 | 0.3401 (4) | 0.4363 (3) | 0.4950 (3) | 0.0514 (8) |
| C16 | 0.4180 (4) | 0.3383 (3) | 0.5131 (3) | 0.0513 (8) |
| C17 | 0.5540 (4) | 0.3219 (3) | 0.4464 (3) | 0.0570 (9) |
| H17 | 0.5950 | 0.3757 | 0.3910 | 0.068* |
| C18 | 0.5658 (5) | 0.1567 (3) | 0.5374 (4) | 0.0750 (12) |
| H18 | 0.6152 | 0.0940 | 0.5452 | 0.090* |
| C19 | 0.4333 (5) | 0.1661 (3) | 0.6073 (3) | 0.0731 (11) |
| H19 | 0.3941 | 0.1112 | 0.6619 | 0.088* |
| C20 | 0.3579 (4) | 0.2580 (3) | 0.5961 (3) | 0.0635 (10) |

| | | | | |
|---|---|---|---|---|
| H20 | 0.2678 | 0.2662 | 0.6438 | 0.076* |
| C21 | 0.6865 (4) | 0.8056 (3) | 0.0890 (3) | 0.0586 (9) |
| C22 | 0.6915 (3) | 0.8914 (3) | 0.0020 (3) | 0.0507 (8) |
| C23 | 0.6572 (4) | 0.8719 (3) | −0.0823 (3) | 0.0639 (10) |
| H23 | 0.6367 | 0.8058 | −0.0831 | 0.077* |
| C24 | 0.6545 (4) | 0.9530 (3) | −0.1641 (3) | 0.0659 (10) |
| H24 | 0.6351 | 0.9412 | −0.2218 | 0.079* |
| C25 | 0.6802 (4) | 1.0505 (3) | −0.1611 (3) | 0.0653 (10) |
| H25 | 0.6748 | 1.1047 | −0.2156 | 0.078* |
| C26 | 0.7141 (4) | 1.0698 (3) | −0.0781 (3) | 0.0577 (9) |
| H26 | 0.7322 | 1.1366 | −0.0778 | 0.069* |
| C27 | 0.7215 (3) | 0.9901 (3) | 0.0050 (3) | 0.0465 (8) |
| C28 | 0.7665 (3) | 1.0123 (2) | 0.0908 (2) | 0.0457 (8) |
| C29 | 0.7080 (3) | 1.0970 (3) | 0.1394 (3) | 0.0510 (8) |
| H29 | 0.6391 | 1.1393 | 0.1195 | 0.061* |
| C30 | 0.7528 (3) | 1.1180 (2) | 0.2172 (3) | 0.0477 (8) |
| H30 | 0.7115 | 1.1732 | 0.2503 | 0.057* |
| C31 | 0.8579 (3) | 1.0579 (2) | 0.2462 (3) | 0.0478 (8) |
| C32 | 0.9173 (4) | 0.9740 (3) | 0.1969 (3) | 0.0523 (8) |
| H32 | 0.9882 | 0.9330 | 0.2153 | 0.063* |
| C33 | 0.8711 (4) | 0.9519 (3) | 0.1210 (3) | 0.0534 (9) |
| H33 | 0.9107 | 0.8954 | 0.0895 | 0.064* |
| C34 | 0.9099 (4) | 1.0827 (2) | 0.3284 (3) | 0.0540 (9) |
| H34A | 1.0023 | 1.1112 | 0.2935 | 0.065* |
| H34B | 0.8469 | 1.1337 | 0.3643 | 0.065* |
| C35 | 0.8588 (4) | 0.8580 (2) | 0.5220 (3) | 0.0466 (8) |
| C36 | 0.7784 (4) | 0.7789 (2) | 0.6086 (2) | 0.0457 (8) |
| C37 | 0.8411 (4) | 0.6860 (3) | 0.6409 (3) | 0.0571 (9) |
| H37 | 0.9364 | 0.6726 | 0.6083 | 0.068* |
| C38 | 0.7600 (4) | 0.6138 (3) | 0.7220 (3) | 0.0641 (10) |
| H38 | 0.8000 | 0.5512 | 0.7459 | 0.077* |
| C39 | 0.6189 (4) | 0.6359 (3) | 0.7673 (3) | 0.0646 (10) |
| H39 | 0.5646 | 0.5857 | 0.8204 | 0.078* |
| C40 | 0.6352 (4) | 0.7937 (3) | 0.6600 (3) | 0.0538 (9) |
| H40 | 0.5927 | 0.8555 | 0.6373 | 0.065* |
| N1 | 0.3591 (3) | 0.4065 (3) | 0.0031 (3) | 0.0677 (9) |
| N2 | 0.3825 (3) | 0.5112 (2) | 0.4104 (2) | 0.0522 (7) |
| N3 | 0.2766 (3) | 0.5798 (2) | 0.4296 (2) | 0.0531 (7) |
| N4 | 0.1736 (3) | 0.5504 (3) | 0.5198 (3) | 0.0775 (10) |
| N5 | 0.2121 (3) | 0.4598 (3) | 0.5637 (3) | 0.0717 (9) |
| N6 | 0.6296 (4) | 0.2346 (3) | 0.4563 (3) | 0.0729 (9) |
| N7 | 0.6834 (4) | 0.7392 (3) | 0.1563 (3) | 0.0806 (10) |
| N8 | 0.8039 (3) | 0.9433 (2) | 0.4788 (2) | 0.0511 (7) |
| N9 | 0.9167 (3) | 0.9889 (2) | 0.4062 (2) | 0.0499 (7) |
| N10 | 1.0358 (3) | 0.9351 (2) | 0.4026 (2) | 0.0596 (8) |
| N11 | 1.0016 (3) | 0.8513 (2) | 0.4766 (2) | 0.0554 (7) |
| N12 | 0.5550 (3) | 0.7260 (2) | 0.7389 (2) | 0.0621 (8) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0432 (18) | 0.058 (2) | 0.052 (2) | −0.0010 (16) | −0.0159 (17) | −0.0213 (17) |
| C2 | 0.0494 (19) | 0.0420 (17) | 0.049 (2) | −0.0119 (15) | −0.0147 (16) | −0.0065 (14) |
| C3 | 0.060 (2) | 0.072 (2) | 0.054 (2) | −0.0023 (19) | −0.0214 (19) | −0.0159 (18) |
| C4 | 0.075 (3) | 0.071 (3) | 0.062 (2) | −0.016 (2) | −0.034 (2) | −0.004 (2) |
| C5 | 0.063 (2) | 0.063 (2) | 0.073 (3) | −0.014 (2) | −0.037 (2) | 0.011 (2) |
| C6 | 0.057 (2) | 0.048 (2) | 0.069 (2) | −0.0036 (17) | −0.026 (2) | −0.0077 (17) |
| C7 | 0.0377 (17) | 0.0425 (17) | 0.054 (2) | −0.0041 (14) | −0.0156 (16) | −0.0054 (15) |
| C8 | 0.0473 (18) | 0.0410 (17) | 0.050 (2) | 0.0017 (14) | −0.0193 (16) | −0.0112 (14) |
| C9 | 0.0398 (17) | 0.0434 (18) | 0.051 (2) | −0.0025 (14) | −0.0103 (15) | −0.0126 (15) |
| C10 | 0.0397 (17) | 0.0470 (18) | 0.059 (2) | −0.0007 (14) | −0.0155 (17) | −0.0130 (16) |
| C11 | 0.0501 (19) | 0.0379 (17) | 0.051 (2) | −0.0005 (15) | −0.0190 (17) | −0.0081 (14) |
| C12 | 0.048 (2) | 0.061 (2) | 0.052 (2) | 0.0051 (17) | −0.0118 (17) | −0.0169 (17) |
| C13 | 0.0389 (18) | 0.058 (2) | 0.062 (2) | 0.0042 (15) | −0.0169 (17) | −0.0194 (17) |
| C14 | 0.065 (2) | 0.0469 (19) | 0.058 (2) | 0.0020 (17) | −0.0252 (19) | −0.0119 (16) |
| C15 | 0.052 (2) | 0.059 (2) | 0.046 (2) | −0.0031 (17) | −0.0192 (17) | −0.0123 (16) |
| C16 | 0.054 (2) | 0.058 (2) | 0.049 (2) | 0.0033 (17) | −0.0238 (18) | −0.0173 (16) |
| C17 | 0.056 (2) | 0.056 (2) | 0.064 (2) | −0.0023 (18) | −0.023 (2) | −0.0172 (18) |
| C18 | 0.086 (3) | 0.061 (3) | 0.082 (3) | 0.010 (2) | −0.034 (3) | −0.019 (2) |
| C19 | 0.089 (3) | 0.057 (2) | 0.070 (3) | 0.001 (2) | −0.029 (3) | −0.005 (2) |
| C20 | 0.067 (2) | 0.060 (2) | 0.059 (2) | −0.0051 (19) | −0.016 (2) | −0.0085 (18) |
| C21 | 0.068 (2) | 0.049 (2) | 0.064 (2) | −0.0112 (19) | −0.025 (2) | −0.0147 (19) |
| C22 | 0.0447 (19) | 0.056 (2) | 0.052 (2) | 0.0004 (16) | −0.0148 (16) | −0.0159 (16) |
| C23 | 0.067 (2) | 0.065 (2) | 0.069 (3) | −0.009 (2) | −0.025 (2) | −0.027 (2) |
| C24 | 0.070 (3) | 0.078 (3) | 0.061 (2) | 0.002 (2) | −0.031 (2) | −0.023 (2) |
| C25 | 0.075 (3) | 0.068 (3) | 0.059 (2) | 0.002 (2) | −0.032 (2) | −0.0097 (19) |
| C26 | 0.064 (2) | 0.053 (2) | 0.060 (2) | 0.0039 (18) | −0.027 (2) | −0.0118 (17) |
| C27 | 0.0409 (17) | 0.054 (2) | 0.048 (2) | −0.0014 (15) | −0.0146 (16) | −0.0164 (15) |
| C28 | 0.0450 (18) | 0.0449 (18) | 0.0462 (19) | −0.0030 (15) | −0.0126 (16) | −0.0112 (14) |
| C29 | 0.0481 (19) | 0.052 (2) | 0.055 (2) | 0.0070 (16) | −0.0214 (17) | −0.0124 (16) |
| C30 | 0.055 (2) | 0.0371 (17) | 0.051 (2) | −0.0034 (15) | −0.0159 (17) | −0.0136 (14) |
| C31 | 0.0505 (19) | 0.0456 (18) | 0.0461 (19) | −0.0065 (15) | −0.0158 (16) | −0.0051 (15) |
| C32 | 0.051 (2) | 0.0496 (19) | 0.061 (2) | 0.0011 (16) | −0.0245 (18) | −0.0132 (16) |
| C33 | 0.053 (2) | 0.050 (2) | 0.062 (2) | 0.0094 (16) | −0.0221 (18) | −0.0230 (17) |
| C34 | 0.068 (2) | 0.0457 (19) | 0.052 (2) | −0.0100 (17) | −0.0259 (19) | −0.0027 (15) |
| C35 | 0.054 (2) | 0.0444 (18) | 0.050 (2) | 0.0071 (16) | −0.0264 (17) | −0.0157 (15) |
| C36 | 0.057 (2) | 0.0447 (18) | 0.0433 (19) | 0.0008 (15) | −0.0248 (17) | −0.0133 (14) |
| C37 | 0.059 (2) | 0.053 (2) | 0.062 (2) | 0.0093 (18) | −0.0262 (19) | −0.0112 (18) |
| C38 | 0.079 (3) | 0.048 (2) | 0.070 (3) | 0.007 (2) | −0.037 (2) | −0.0068 (18) |
| C39 | 0.075 (3) | 0.062 (2) | 0.058 (2) | −0.006 (2) | −0.027 (2) | −0.0074 (18) |
| C40 | 0.062 (2) | 0.050 (2) | 0.053 (2) | 0.0082 (17) | −0.0256 (19) | −0.0136 (16) |
| N1 | 0.061 (2) | 0.078 (2) | 0.074 (2) | 0.0183 (17) | −0.0294 (18) | −0.0337 (18) |
| N2 | 0.0522 (17) | 0.0555 (17) | 0.0503 (18) | 0.0062 (14) | −0.0181 (14) | −0.0168 (14) |
| N3 | 0.0519 (17) | 0.0600 (18) | 0.0489 (18) | 0.0058 (15) | −0.0190 (15) | −0.0148 (14) |
| N4 | 0.061 (2) | 0.083 (2) | 0.067 (2) | 0.0175 (18) | −0.0082 (19) | −0.0046 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N5 | 0.057 (2) | 0.072 (2) | 0.066 (2) | 0.0097 (17) | −0.0089 (17) | 0.0003 (17) |
| N6 | 0.074 (2) | 0.073 (2) | 0.075 (2) | 0.0214 (19) | −0.0280 (19) | −0.0305 (19) |
| N7 | 0.112 (3) | 0.062 (2) | 0.076 (2) | −0.022 (2) | −0.039 (2) | −0.0089 (18) |
| N8 | 0.0549 (17) | 0.0446 (15) | 0.0557 (18) | 0.0006 (13) | −0.0225 (15) | −0.0089 (13) |
| N9 | 0.0531 (17) | 0.0520 (16) | 0.0482 (17) | 0.0003 (14) | −0.0219 (15) | −0.0105 (13) |
| N10 | 0.0548 (18) | 0.072 (2) | 0.0533 (18) | 0.0049 (16) | −0.0218 (15) | −0.0122 (16) |
| N11 | 0.0589 (19) | 0.0517 (17) | 0.0562 (19) | 0.0051 (14) | −0.0252 (16) | −0.0062 (14) |
| N12 | 0.0614 (19) | 0.062 (2) | 0.058 (2) | −0.0027 (16) | −0.0157 (17) | −0.0101 (16) |

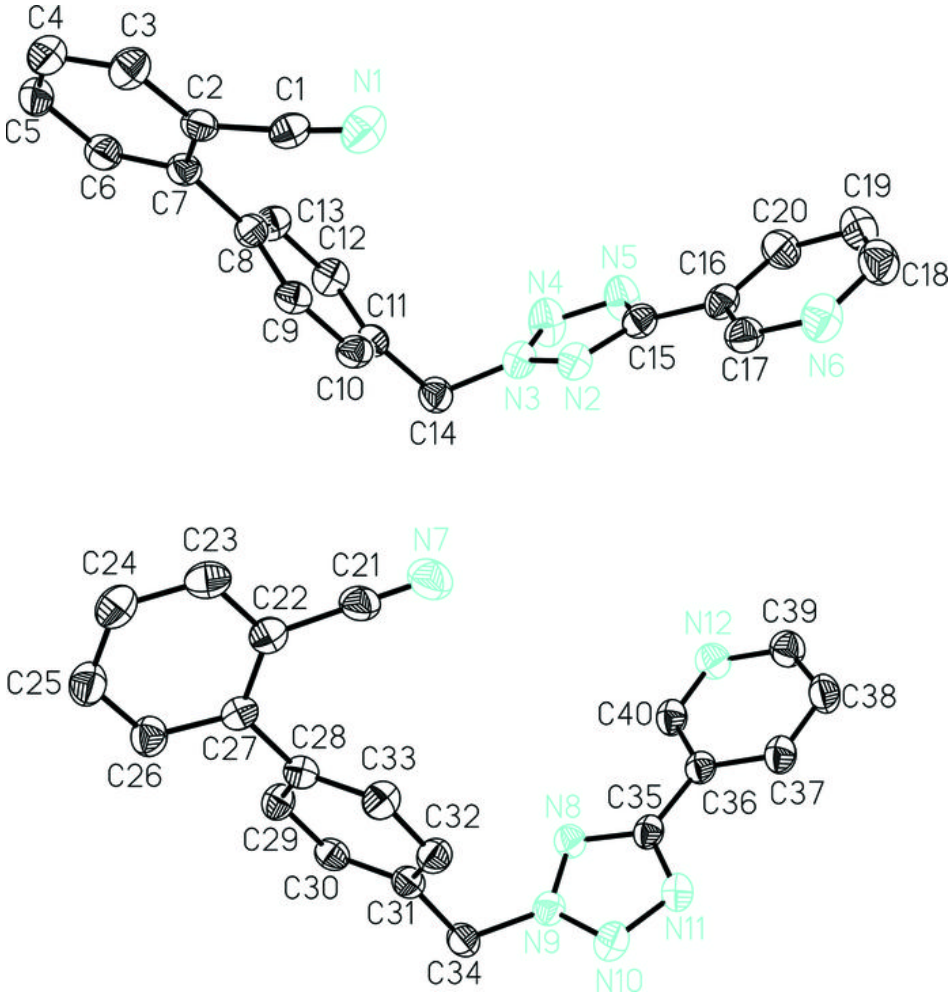
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.153 (4) | C22—C23 | 1.404 (5) |
| C1—C2 | 1.437 (5) | C23—C24 | 1.379 (5) |
| C2—C3 | 1.391 (4) | C23—H23 | 0.9300 |
| C2—C7 | 1.407 (4) | C24—C25 | 1.364 (5) |
| C3—C4 | 1.359 (5) | C24—H24 | 0.9300 |
| C3—H3 | 0.9300 | C25—C26 | 1.382 (5) |
| C4—C5 | 1.385 (5) | C25—H25 | 0.9300 |
| C4—H4 | 0.9300 | C26—C27 | 1.392 (4) |
| C5—C6 | 1.384 (5) | C26—H26 | 0.9300 |
| C5—H5 | 0.9300 | C27—C28 | 1.501 (4) |
| C6—C7 | 1.387 (4) | C28—C33 | 1.391 (4) |
| C6—H6 | 0.9300 | C28—C29 | 1.402 (4) |
| C7—C8 | 1.499 (4) | C29—C30 | 1.391 (4) |
| C8—C13 | 1.381 (4) | C29—H29 | 0.9300 |
| C8—C9 | 1.395 (4) | C30—C31 | 1.385 (4) |
| C9—C10 | 1.391 (4) | C30—H30 | 0.9300 |
| C9—H9 | 0.9300 | C31—C32 | 1.400 (4) |
| C10—C11 | 1.377 (4) | C31—C34 | 1.513 (4) |
| C10—H10 | 0.9300 | C32—C33 | 1.382 (4) |
| C11—C12 | 1.395 (4) | C32—H32 | 0.9300 |
| C11—C14 | 1.505 (4) | C33—H33 | 0.9300 |
| C12—C13 | 1.391 (4) | C34—N9 | 1.465 (4) |
| C12—H12 | 0.9300 | C34—H34A | 0.9700 |
| C13—H13 | 0.9300 | C34—H34B | 0.9700 |
| C14—N3 | 1.460 (4) | C35—N8 | 1.324 (4) |
| C14—H14A | 0.9700 | C35—N11 | 1.366 (4) |
| C14—H14B | 0.9700 | C35—C36 | 1.462 (5) |
| C15—N2 | 1.324 (4) | C36—C37 | 1.385 (4) |
| C15—N5 | 1.361 (4) | C36—C40 | 1.390 (5) |
| C15—C16 | 1.469 (5) | C37—C38 | 1.376 (5) |
| C16—C20 | 1.387 (5) | C37—H37 | 0.9300 |
| C16—C17 | 1.387 (5) | C38—C39 | 1.376 (5) |
| C17—N6 | 1.329 (4) | C38—H38 | 0.9300 |
| C17—H17 | 0.9300 | C39—N12 | 1.346 (4) |
| C18—C19 | 1.361 (6) | C39—H39 | 0.9300 |
| C18—N6 | 1.364 (5) | C40—N12 | 1.326 (4) |
| C18—H18 | 0.9300 | C40—H40 | 0.9300 |
| C19—C20 | 1.379 (5) | N2—N3 | 1.323 (3) |

| | | | |
|---|---|---|---|
| C19—H19 | 0.9300 | N3—N4 | 1.319 (4) |
| C20—H20 | 0.9300 | N4—N5 | 1.308 (4) |
| C21—N7 | 1.122 (4) | N8—N9 | 1.326 (4) |
| C21—C22 | 1.448 (5) | N9—N10 | 1.330 (4) |
| C22—C27 | 1.394 (4) | N10—N11 | 1.316 (4) |
| N1—C1—C2 | 176.0 (3) | C25—C24—C23 | 120.6 (4) |
| C3—C2—C7 | 120.7 (3) | C25—C24—H24 | 119.7 |
| C3—C2—C1 | 118.2 (3) | C23—C24—H24 | 119.7 |
| C7—C2—C1 | 121.0 (3) | C24—C25—C26 | 120.9 (4) |
| C4—C3—C2 | 120.9 (4) | C24—C25—H25 | 119.5 |
| C4—C3—H3 | 119.6 | C26—C25—H25 | 119.5 |
| C2—C3—H3 | 119.6 | C25—C26—C27 | 120.6 (3) |
| C3—C4—C5 | 119.6 (4) | C25—C26—H26 | 119.7 |
| C3—C4—H4 | 120.2 | C27—C26—H26 | 119.7 |
| C5—C4—H4 | 120.2 | C26—C27—C22 | 117.7 (3) |
| C6—C5—C4 | 119.9 (4) | C26—C27—C28 | 119.4 (3) |
| C6—C5—H5 | 120.0 | C22—C27—C28 | 122.9 (3) |
| C4—C5—H5 | 120.0 | C33—C28—C29 | 118.4 (3) |
| C5—C6—C7 | 121.9 (4) | C33—C28—C27 | 120.8 (3) |
| C5—C6—H6 | 119.0 | C29—C28—C27 | 120.7 (3) |
| C7—C6—H6 | 119.0 | C30—C29—C28 | 120.1 (3) |
| C6—C7—C2 | 116.9 (3) | C30—C29—H29 | 119.9 |
| C6—C7—C8 | 121.5 (3) | C28—C29—H29 | 119.9 |
| C2—C7—C8 | 121.7 (3) | C31—C30—C29 | 121.1 (3) |
| C13—C8—C9 | 118.1 (3) | C31—C30—H30 | 119.5 |
| C13—C8—C7 | 121.8 (3) | C29—C30—H30 | 119.5 |
| C9—C8—C7 | 120.1 (3) | C30—C31—C32 | 118.7 (3) |
| C10—C9—C8 | 120.9 (3) | C30—C31—C34 | 121.1 (3) |
| C10—C9—H9 | 119.6 | C32—C31—C34 | 120.1 (3) |
| C8—C9—H9 | 119.6 | C33—C32—C31 | 120.3 (3) |
| C11—C10—C9 | 121.1 (3) | C33—C32—H32 | 119.9 |
| C11—C10—H10 | 119.4 | C31—C32—H32 | 119.9 |
| C9—C10—H10 | 119.4 | C32—C33—C28 | 121.3 (3) |
| C10—C11—C12 | 118.0 (3) | C32—C33—H33 | 119.3 |
| C10—C11—C14 | 120.7 (3) | C28—C33—H33 | 119.3 |
| C12—C11—C14 | 121.3 (3) | N9—C34—C31 | 109.9 (3) |
| C13—C12—C11 | 121.1 (3) | N9—C34—H34A | 109.7 |
| C13—C12—H12 | 119.5 | C31—C34—H34A | 109.7 |
| C11—C12—H12 | 119.5 | N9—C34—H34B | 109.7 |
| C8—C13—C12 | 120.8 (3) | C31—C34—H34B | 109.7 |
| C8—C13—H13 | 119.6 | H34A—C34—H34B | 108.2 |
| C12—C13—H13 | 119.6 | N8—C35—N11 | 112.3 (3) |
| N3—C14—C11 | 113.6 (3) | N8—C35—C36 | 124.8 (3) |
| N3—C14—H14A | 108.8 | N11—C35—C36 | 122.9 (3) |
| C11—C14—H14A | 108.8 | C37—C36—C40 | 117.6 (3) |
| N3—C14—H14B | 108.8 | C37—C36—C35 | 121.4 (3) |
| C11—C14—H14B | 108.8 | C40—C36—C35 | 121.0 (3) |
| H14A—C14—H14B | 107.7 | C38—C37—C36 | 119.0 (3) |
| N2—C15—N5 | 111.6 (3) | C38—C37—H37 | 120.5 |

| | | | |
|---|---|---|---|
| N2—C15—C16 | 125.2 (3) | C36—C37—H37 | 120.5 |
| N5—C15—C16 | 123.2 (3) | C39—C38—C37 | 118.8 (3) |
| C20—C16—C17 | 117.4 (3) | C39—C38—H38 | 120.6 |
| C20—C16—C15 | 121.5 (3) | C37—C38—H38 | 120.6 |
| C17—C16—C15 | 121.1 (3) | N12—C39—C38 | 123.7 (4) |
| N6—C17—C16 | 124.4 (4) | N12—C39—H39 | 118.1 |
| N6—C17—H17 | 117.8 | C38—C39—H39 | 118.1 |
| C16—C17—H17 | 117.8 | N12—C40—C36 | 124.7 (3) |
| C19—C18—N6 | 123.2 (4) | N12—C40—H40 | 117.7 |
| C19—C18—H18 | 118.4 | C36—C40—H40 | 117.6 |
| N6—C18—H18 | 118.4 | C15—N2—N3 | 102.3 (3) |
| C18—C19—C20 | 119.2 (4) | N4—N3—N2 | 113.4 (3) |
| C18—C19—H19 | 120.4 | N4—N3—C14 | 122.7 (3) |
| C20—C19—H19 | 120.4 | N2—N3—C14 | 123.8 (3) |
| C19—C20—C16 | 119.3 (4) | N5—N4—N3 | 106.7 (3) |
| C19—C20—H20 | 120.3 | N4—N5—C15 | 106.0 (3) |
| C16—C20—H20 | 120.3 | C17—N6—C18 | 116.4 (4) |
| N7—C21—C22 | 179.6 (4) | C35—N8—N9 | 102.1 (3) |
| C27—C22—C23 | 121.6 (3) | N8—N9—N10 | 113.6 (3) |
| C27—C22—C21 | 121.3 (3) | N8—N9—C34 | 123.2 (3) |
| C23—C22—C21 | 117.0 (3) | N10—N9—C34 | 122.8 (3) |
| C24—C23—C22 | 118.5 (3) | N11—N10—N9 | 106.5 (3) |
| C24—C23—H23 | 120.7 | N10—N11—C35 | 105.6 (3) |
| C22—C23—H23 | 120.7 | C40—N12—C39 | 116.1 (3) |

**Fig. 1**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