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# (*Z*)-Amino(2-methyl-3-oxoisoindolin-1-ylidene)acetonitrile

**Dieter Schollmeyer,[a] Dorota Ferenc[a] and Till Opatz[b]***

[a]Institut für Organische Chemie, Universität Mainz, Duesbergweg 10-14, 55128 Mainz, Germany, and [b]Department Chemie, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany
Correspondence e-mail: opatz@chemie.uni-hamburg.de

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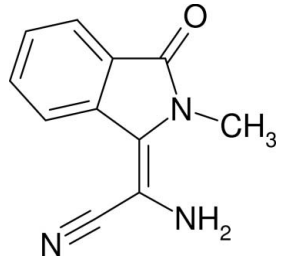
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.047; $wR$ factor = 0.114; data-to-parameter ratio = 16.7.

The asymmetric unit of the title compound, $C_{11}H_9N_3O$, contains two independent and nearly identical molecules (*A* and *B*). Molecule *A* can be transformed to *B* using a rotation of approximately 85° around the [111] direction. Each *A* molecule is connected to three *B* molecules *via* N—H···N and N—H···O hydrogen bonds and *vice versa*. Centrosymmetrically related molecules of the same residue form $\pi$–$\pi$ interactions with centroid–centroid distances of 4.326 (1) and 3.826 (1) Å for the benzene rings of molecules *A* and *B*, respectively.

## Related literature

For the preparation of the compound as well as the crystal structure of the corresponding 2-benzyl derivative, see: Opatz & Ferenc (2004). For the crystal structure of the distantly related compound *N*-(2-amino-1,2-dicyanovinyl)acetamide, see: Al-Azmi *et al.*, (2001).




## Experimental

### Crystal data

$C_{11}H_9N_3O$
$M_r$ = 199.21
Triclinic, $P\overline{1}$
$a$ = 8.5021 (7) Å
$b$ = 8.5080 (6) Å
$c$ = 14.0412 (11) Å
$\alpha$ = 80.741 (5)°
$\beta$ = 80.797 (5)°
$\gamma$ = 68.329 (4)°
$V$ = 925.98 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 298 K
0.44 × 0.30 × 0.24 mm

### Data collection

Bruker SMART APEXII diffractometer
Absorption correction: none
13710 measured reflections
4570 independent reflections
3668 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.095

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
$S$ = 0.97
4570 reflections
274 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N13*A*—H13*A*···N15*B*$^{i}$ | 0.97 | 2.08 | 3.035 (3) | 169 |
| N13*B*—H13*C*···O10*A*$^{ii}$ | 0.94 | 2.04 | 2.948 (2) | 163 |
| N13*B*—H13*D*···N13*A*$^{iii}$ | 0.97 | 2.52 | 3.238 (3) | 131 |

Symmetry codes: (i) $x, y-1, z-1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y, z+1$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5125).

## References

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# supporting information

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## (*Z*)-Amino(2-methyl-3-oxoisoindolin-1-ylidene)acetonitrile

**Dieter Schollmeyer, Dorota Ferenc and Till Opatz**

### S1. Comment

Amino(2-alkyl-3-oxo-2,3-dihydro-1*H*-isoindol-1-ylidene)acetonitriles are readily obtained in a three-component reaction between 2-carboxybenzaldehyde (2-formylbenzoic acid), aliphatic amines and cyanide in acidic medium. While steric hindrance is a decisive factor and the reaction fails for $\alpha$-branched primary amines such as isopropylamine, all tested unbranched primary amines give the desired products. Consequently, the highest yield of 53% is found for the preparation of the title compound, in which unfavorable steric interactions are reduced to a minimum. Despite the fact that this compound had been obtained as the prototype example of the series, the determination of its crystal structure was hampered by twinning of the crystals. Compared to the *N*-benzyl derivative described earlier (Opatz & Ferenc, 2004), the exocyclic aminoacetonitrile unit is even less twisted against the plane of the bicyclic $\pi$-system (5.0 (1)° and 1.7 (2)°) (Fig. 1). Furthermore, the compound forms a hydrogen bonded network, in which both exocyclic nitrogen atoms as well as the oxygen atom act as acceptors and the $NH_2$ group is the double donor. Centrosymetrically related molecules of the same residue form $\pi$-$\pi$-interactions. The distances between the centroids are 4.326 (1)Å and 3.826 (1)Å for the rings C1–C6 of A and B respectively (Fig. 2).

### S2. Experimental

The preparation was carried out as described in the procedure reported by Opatz and Ferenc (2004). The (*Z*)-isomer was obtained by recrystallization of the isomeric mixture from hexanes/ethyl acetate. Single crystals suitable for X-ray crystallography were grown by evaporation from a $CH_2Cl_2$ solution.

### S3. Refinement

Hydrogen atoms attached to carbons were placed at calculated positions with C—H = 0.95 Å (aromatic) or 0.98–0.99 Å ($sp^3$ C-atom). Hydrogen atoms attached to N were located in difference Fourier maps. All H atoms were refined in the riding-model approximation with isotropic displacement parameters (set at 1.2–1.5 times of the $U_{eq}$ of the parent atom). The crystal used for data collection was twinned. Using the twin matrix 0 - 1 0, -1 0 0, 0 0 - 1 with BSAF 0.468 (1) the structure refinement was succesful.

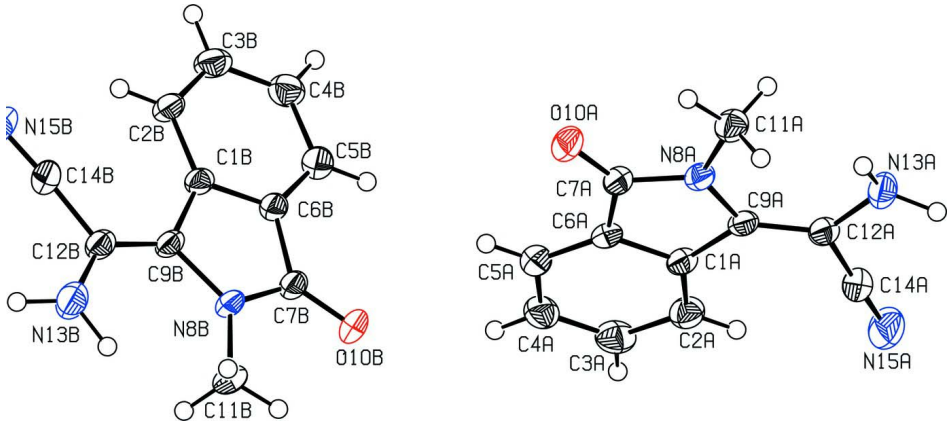


**Figure 1**

View of compound **I**. Displacement ellipsoids are drawn at the 50% probability level.

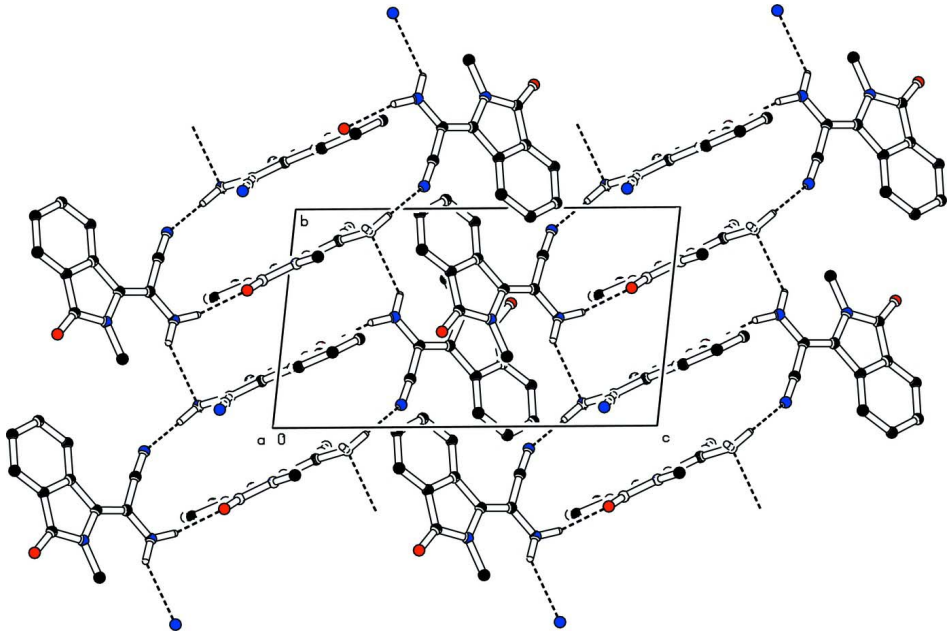


**Figure 2**

Part of the packing diagram. Hydrogen bonds with dashed lines.

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*Crystal data*

$C_{11}H_9N_3O$
$M_r = 199.21$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.5021\ (7)$ Å
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$c = 14.0412\ (11)$ Å
$\alpha = 80.741\ (5)°$
$\beta = 80.797\ (5)°$
$\gamma = 68.329\ (4)°$
$V = 925.98\ (12)$ Å$^3$
$Z = 4$
$F(000) = 416$
$D_x = 1.429$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5592 reflections
$\theta = 2.5–27.8°$
$\mu = 0.10$ mm$^{-1}$
$T = 298$ K
Block, yellow
0.44 × 0.30 × 0.24 mm

*Data collection*

Bruker SMART APEXII diffractometer
Radiation source: sealed tube
Graphite monochromator
CCD scan
13710 measured reflections
4570 independent reflections
3668 reflections with $I > 2\sigma(I)$
$R_{int} = 0.095$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.6°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.114$
$S = 0.97$
4570 reflections
274 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1A | 0.2396 (3) | 0.2747 (2) | 0.03598 (13) | 0.0253 (4) |
| C2A | 0.0717 (3) | 0.2796 (3) | 0.05168 (15) | 0.0336 (5) |
| H2A | 0.0273 | 0.2403 | 0.0079 | 0.040* |
| C3A | −0.0270 (3) | 0.3451 (3) | 0.13471 (15) | 0.0383 (5) |
| H3A | −0.1390 | 0.3487 | 0.1464 | 0.046* |
| C4A | 0.0353 (3) | 0.4049 (3) | 0.20035 (15) | 0.0368 (5) |
| H4A | −0.0345 | 0.4474 | 0.2554 | 0.044* |
| C5A | 0.2019 (3) | 0.4024 (2) | 0.18496 (14) | 0.0331 (4) |
| H5A | 0.2454 | 0.4423 | 0.2289 | 0.040* |
| C6A | 0.3004 (3) | 0.3385 (2) | 0.10205 (13) | 0.0269 (4) |
| C7A | 0.4779 (3) | 0.3235 (2) | 0.06796 (13) | 0.0270 (4) |
| N8A | 0.5196 (2) | 0.2477 (2) | −0.01665 (11) | 0.0260 (3) |
| C9A | 0.3809 (2) | 0.2157 (2) | −0.04199 (13) | 0.0244 (4) |
| O10A | 0.5747 (2) | 0.36850 (19) | 0.10405 (10) | 0.0367 (3) |
| C11A | 0.6877 (3) | 0.2169 (3) | −0.07052 (14) | 0.0334 (5) |
| H11A | 0.7539 | 0.2569 | −0.0375 | 0.050* |
| H11B | 0.6761 | 0.2765 | −0.1346 | 0.050* |

| | | | | |
|---|---|---|---|---|
| H11C | 0.7439 | 0.0971 | −0.0749 | 0.050* |
| C12A | 0.3794 (3) | 0.1446 (2) | −0.12086 (13) | 0.0274 (4) |
| N13A | 0.5046 (2) | 0.1033 (2) | −0.19937 (12) | 0.0378 (4) |
| H13A | 0.4929 | 0.0314 | −0.2428 | 0.057* |
| H13B | 0.6248 | 0.0872 | −0.1858 | 0.057* |
| C14A | 0.2264 (3) | 0.1156 (3) | −0.13240 (14) | 0.0333 (5) |
| N15A | 0.1094 (3) | 0.0862 (3) | −0.14296 (14) | 0.0497 (5) |
| C1B | 0.2361 (2) | 0.7692 (2) | 0.48593 (13) | 0.0255 (4) |
| C2B | 0.2327 (3) | 0.9368 (2) | 0.46907 (14) | 0.0315 (5) |
| H2B | 0.2776 | 0.9793 | 0.5111 | 0.038* |
| C3B | 0.1607 (3) | 1.0388 (3) | 0.38784 (15) | 0.0365 (5) |
| H3B | 0.1575 | 1.1506 | 0.3760 | 0.044* |
| C4B | 0.0932 (3) | 0.9777 (3) | 0.32407 (15) | 0.0364 (5) |
| H4B | 0.0454 | 1.0487 | 0.2706 | 0.044* |
| C5B | 0.0971 (3) | 0.8124 (3) | 0.33976 (14) | 0.0340 (5) |
| H5B | 0.0527 | 0.7702 | 0.2975 | 0.041* |
| C6B | 0.1689 (3) | 0.7110 (2) | 0.42024 (13) | 0.0273 (4) |
| C7B | 0.1883 (3) | 0.5323 (2) | 0.45288 (13) | 0.0285 (4) |
| N8B | 0.2650 (2) | 0.49057 (19) | 0.53725 (11) | 0.0283 (4) |
| C9B | 0.2977 (2) | 0.6286 (2) | 0.56289 (13) | 0.0257 (4) |
| O10B | 0.1472 (2) | 0.43614 (19) | 0.41427 (10) | 0.0382 (4) |
| C11B | 0.2984 (3) | 0.3212 (2) | 0.58994 (15) | 0.0356 (5) |
| H11D | 0.2602 | 0.2548 | 0.5561 | 0.053* |
| H11E | 0.2386 | 0.3306 | 0.6540 | 0.053* |
| H11F | 0.4184 | 0.2667 | 0.5944 | 0.053* |
| C12B | 0.3717 (3) | 0.6276 (2) | 0.64150 (14) | 0.0285 (4) |
| N13B | 0.4376 (3) | 0.4959 (2) | 0.71336 (13) | 0.0409 (4) |
| H13C | 0.4549 | 0.5204 | 0.7730 | 0.061* |
| H13D | 0.4177 | 0.3943 | 0.7053 | 0.061* |
| C14B | 0.3965 (3) | 0.7805 (3) | 0.65574 (14) | 0.0334 (4) |
| N15B | 0.4204 (3) | 0.8972 (3) | 0.67200 (14) | 0.0483 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1A | 0.0268 (10) | 0.0205 (9) | 0.0297 (9) | −0.0101 (8) | −0.0021 (7) | −0.0029 (7) |
| C2A | 0.0313 (12) | 0.0356 (11) | 0.0376 (10) | −0.0165 (10) | −0.0019 (9) | −0.0049 (9) |
| C3A | 0.0289 (12) | 0.0403 (12) | 0.0448 (12) | −0.0153 (9) | 0.0048 (9) | −0.0037 (9) |
| C4A | 0.0401 (12) | 0.0329 (11) | 0.0346 (10) | −0.0133 (9) | 0.0080 (9) | −0.0067 (9) |
| C5A | 0.0417 (13) | 0.0291 (10) | 0.0306 (10) | −0.0159 (9) | 0.0012 (9) | −0.0059 (8) |
| C6A | 0.0340 (11) | 0.0199 (9) | 0.0292 (9) | −0.0135 (8) | −0.0020 (8) | −0.0011 (7) |
| C7A | 0.0326 (10) | 0.0240 (9) | 0.0273 (9) | −0.0128 (8) | −0.0046 (8) | −0.0026 (7) |
| N8A | 0.0269 (9) | 0.0262 (8) | 0.0288 (7) | −0.0139 (7) | −0.0008 (6) | −0.0047 (6) |
| C9A | 0.0278 (10) | 0.0203 (9) | 0.0276 (9) | −0.0120 (8) | −0.0032 (7) | −0.0006 (7) |
| O10A | 0.0405 (9) | 0.0431 (8) | 0.0372 (7) | −0.0240 (7) | −0.0049 (6) | −0.0111 (6) |
| C11A | 0.0295 (11) | 0.0376 (11) | 0.0373 (11) | −0.0169 (9) | 0.0020 (8) | −0.0095 (9) |
| C12A | 0.0324 (11) | 0.0239 (9) | 0.0281 (9) | −0.0127 (8) | −0.0047 (8) | −0.0011 (7) |
| N13A | 0.0425 (11) | 0.0443 (11) | 0.0347 (9) | −0.0227 (9) | 0.0054 (8) | −0.0183 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14A | 0.0397 (12) | 0.0357 (11) | 0.0288 (9) | −0.0171 (10) | −0.0050 (8) | −0.0054 (8) |
| N15A | 0.0510 (13) | 0.0666 (14) | 0.0468 (11) | −0.0343 (11) | −0.0064 (9) | −0.0153 (10) |
| C1B | 0.0258 (10) | 0.0236 (9) | 0.0286 (9) | −0.0122 (8) | 0.0058 (7) | −0.0078 (7) |
| C2B | 0.0379 (12) | 0.0260 (10) | 0.0358 (10) | −0.0179 (9) | 0.0021 (9) | −0.0082 (8) |
| C3B | 0.0420 (12) | 0.0244 (10) | 0.0425 (11) | −0.0148 (9) | 0.0040 (9) | −0.0034 (8) |
| C4B | 0.0419 (13) | 0.0308 (11) | 0.0345 (10) | −0.0130 (10) | −0.0013 (9) | 0.0001 (8) |
| C5B | 0.0379 (12) | 0.0370 (11) | 0.0313 (10) | −0.0183 (10) | 0.0010 (8) | −0.0079 (8) |
| C6B | 0.0316 (11) | 0.0269 (9) | 0.0265 (9) | −0.0153 (8) | 0.0052 (7) | −0.0083 (7) |
| C7B | 0.0337 (11) | 0.0263 (10) | 0.0296 (9) | −0.0159 (8) | 0.0056 (8) | −0.0111 (7) |
| N8B | 0.0372 (10) | 0.0213 (8) | 0.0313 (8) | −0.0159 (7) | 0.0017 (7) | −0.0081 (6) |
| C9B | 0.0273 (10) | 0.0208 (9) | 0.0317 (9) | −0.0118 (8) | 0.0038 (7) | −0.0098 (7) |
| O10B | 0.0548 (10) | 0.0354 (8) | 0.0357 (7) | −0.0260 (8) | −0.0021 (6) | −0.0137 (6) |
| C11B | 0.0492 (13) | 0.0227 (10) | 0.0393 (10) | −0.0184 (9) | −0.0031 (9) | −0.0038 (8) |
| C12B | 0.0296 (10) | 0.0250 (10) | 0.0332 (10) | −0.0123 (8) | 0.0029 (8) | −0.0095 (7) |
| N13B | 0.0592 (13) | 0.0316 (10) | 0.0369 (9) | −0.0181 (9) | −0.0131 (9) | −0.0052 (8) |
| C14B | 0.0392 (12) | 0.0346 (11) | 0.0320 (10) | −0.0171 (9) | −0.0033 (8) | −0.0100 (8) |
| N15B | 0.0668 (14) | 0.0387 (11) | 0.0526 (11) | −0.0287 (10) | −0.0115 (10) | −0.0127 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1A—C2A | 1.395 (3) | C1B—C6B | 1.395 (3) |
| C1A—C6A | 1.395 (3) | C1B—C2B | 1.398 (3) |
| C1A—C9A | 1.485 (2) | C1B—C9B | 1.475 (3) |
| C2A—C3A | 1.387 (3) | C2B—C3B | 1.393 (3) |
| C2A—H2A | 0.9300 | C2B—H2B | 0.9300 |
| C3A—C4A | 1.377 (3) | C3B—C4B | 1.391 (3) |
| C3A—H3A | 0.9300 | C3B—H3B | 0.9300 |
| C4A—C5A | 1.391 (3) | C4B—C5B | 1.377 (3) |
| C4A—H4A | 0.9300 | C4B—H4B | 0.9300 |
| C5A—C6A | 1.381 (3) | C5B—C6B | 1.383 (3) |
| C5A—H5A | 0.9300 | C5B—H5B | 0.9300 |
| C6A—C7A | 1.473 (3) | C6B—C7B | 1.471 (3) |
| C7A—O10A | 1.228 (2) | C7B—O10B | 1.225 (2) |
| C7A—N8A | 1.377 (2) | C7B—N8B | 1.377 (3) |
| N8A—C9A | 1.412 (2) | N8B—C9B | 1.412 (2) |
| N8A—C11A | 1.458 (2) | N8B—C11B | 1.458 (2) |
| C9A—C12A | 1.348 (3) | C9B—C12B | 1.352 (3) |
| C11A—H11A | 0.9600 | C11B—H11D | 0.9600 |
| C11A—H11B | 0.9600 | C11B—H11E | 0.9600 |
| C11A—H11C | 0.9600 | C11B—H11F | 0.9600 |
| C12A—N13A | 1.395 (2) | C12B—N13B | 1.393 (3) |
| C12A—C14A | 1.447 (3) | C12B—C14B | 1.441 (2) |
| N13A—H13A | 0.9688 | N13B—H13C | 0.9399 |
| N13A—H13B | 1.0251 | N13B—H13D | 0.9669 |
| C14A—N15A | 1.148 (3) | C14B—N15B | 1.147 (3) |
| | | | |
| C2A—C1A—C6A | 119.47 (17) | C6B—C1B—C2B | 118.63 (19) |
| C2A—C1A—C9A | 133.57 (17) | C6B—C1B—C9B | 107.85 (15) |

| | | | |
|---|---|---|---|
| C6A—C1A—C9A | 106.95 (16) | C2B—C1B—C9B | 133.53 (18) |
| C3A—C2A—C1A | 117.81 (19) | C3B—C2B—C1B | 118.40 (18) |
| C3A—C2A—H2A | 121.1 | C3B—C2B—H2B | 120.8 |
| C1A—C2A—H2A | 121.1 | C1B—C2B—H2B | 120.8 |
| C4A—C3A—C2A | 122.2 (2) | C4B—C3B—C2B | 121.68 (18) |
| C4A—C3A—H3A | 118.9 | C4B—C3B—H3B | 119.2 |
| C2A—C3A—H3A | 118.9 | C2B—C3B—H3B | 119.2 |
| C3A—C4A—C5A | 120.48 (19) | C5B—C4B—C3B | 120.3 (2) |
| C3A—C4A—H4A | 119.8 | C5B—C4B—H4B | 119.9 |
| C5A—C4A—H4A | 119.8 | C3B—C4B—H4B | 119.9 |
| C6A—C5A—C4A | 117.56 (19) | C4B—C5B—C6B | 118.06 (19) |
| C6A—C5A—H5A | 121.2 | C4B—C5B—H5B | 121.0 |
| C4A—C5A—H5A | 121.2 | C6B—C5B—H5B | 121.0 |
| C5A—C6A—C1A | 122.42 (18) | C5B—C6B—C1B | 122.93 (17) |
| C5A—C6A—C7A | 128.57 (17) | C5B—C6B—C7B | 128.61 (17) |
| C1A—C6A—C7A | 109.01 (16) | C1B—C6B—C7B | 108.46 (17) |
| O10A—C7A—N8A | 124.46 (18) | O10B—C7B—N8B | 125.50 (18) |
| O10A—C7A—C6A | 129.24 (18) | O10B—C7B—C6B | 128.30 (19) |
| N8A—C7A—C6A | 106.30 (15) | N8B—C7B—C6B | 106.20 (14) |
| C7A—N8A—C9A | 111.70 (15) | C7B—N8B—C9B | 112.07 (15) |
| C7A—N8A—C11A | 120.31 (15) | C7B—N8B—C11B | 119.95 (14) |
| C9A—N8A—C11A | 127.93 (15) | C9B—N8B—C11B | 127.95 (16) |
| C12A—C9A—N8A | 126.48 (17) | C12B—C9B—N8B | 126.16 (17) |
| C12A—C9A—C1A | 127.51 (17) | C12B—C9B—C1B | 128.42 (16) |
| N8A—C9A—C1A | 106.01 (14) | N8B—C9B—C1B | 105.42 (15) |
| N8A—C11A—H11A | 109.5 | N8B—C11B—H11D | 109.5 |
| N8A—C11A—H11B | 109.5 | N8B—C11B—H11E | 109.5 |
| H11A—C11A—H11B | 109.5 | H11D—C11B—H11E | 109.5 |
| N8A—C11A—H11C | 109.5 | N8B—C11B—H11F | 109.5 |
| H11A—C11A—H11C | 109.5 | H11D—C11B—H11F | 109.5 |
| H11B—C11A—H11C | 109.5 | H11E—C11B—H11F | 109.5 |
| C9A—C12A—N13A | 128.35 (17) | C9B—C12B—N13B | 130.12 (17) |
| C9A—C12A—C14A | 118.38 (17) | C9B—C12B—C14B | 118.57 (18) |
| N13A—C12A—C14A | 113.12 (16) | N13B—C12B—C14B | 111.26 (17) |
| C12A—N13A—H13A | 116.8 | C12B—N13B—H13C | 120.2 |
| C12A—N13A—H13B | 115.0 | C12B—N13B—H13D | 111.4 |
| H13A—N13A—H13B | 118.1 | H13C—N13B—H13D | 123.8 |
| N15A—C14A—C12A | 177.1 (2) | N15B—C14B—C12B | 175.9 (2) |

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| C6A—C1A—C2A—C3A | −1.5 (3) | C6B—C1B—C2B—C3B | 0.7 (3) |
| C9A—C1A—C2A—C3A | −179.98 (19) | C9B—C1B—C2B—C3B | −178.89 (19) |
| C1A—C2A—C3A—C4A | 0.4 (3) | C1B—C2B—C3B—C4B | −0.1 (3) |
| C2A—C3A—C4A—C5A | 0.3 (3) | C2B—C3B—C4B—C5B | −0.3 (3) |
| C3A—C4A—C5A—C6A | 0.1 (3) | C3B—C4B—C5B—C6B | 0.2 (3) |
| C4A—C5A—C6A—C1A | −1.3 (3) | C4B—C5B—C6B—C1B | 0.4 (3) |
| C4A—C5A—C6A—C7A | 179.10 (18) | C4B—C5B—C6B—C7B | 179.96 (19) |
| C2A—C1A—C6A—C5A | 2.1 (3) | C2B—C1B—C6B—C5B | −0.9 (3) |
| C9A—C1A—C6A—C5A | −179.10 (16) | C9B—C1B—C6B—C5B | 178.83 (17) |

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| C2A—C1A—C6A—C7A | −178.31 (16) | C2B—C1B—C6B—C7B | 179.50 (16) |
| C9A—C1A—C6A—C7A | 0.5 (2) | C9B—C1B—C6B—C7B | −0.8 (2) |
| C5A—C6A—C7A—O10A | −2.3 (3) | C5B—C6B—C7B—O10B | 1.3 (3) |
| C1A—C6A—C7A—O10A | 178.13 (19) | C1B—C6B—C7B—O10B | −179.04 (19) |
| C5A—C6A—C7A—N8A | 178.35 (18) | C5B—C6B—C7B—N8B | −179.13 (19) |
| C1A—C6A—C7A—N8A | −1.3 (2) | C1B—C6B—C7B—N8B | 0.5 (2) |
| O10A—C7A—N8A—C9A | −177.91 (18) | O10B—C7B—N8B—C9B | 179.60 (18) |
| C6A—C7A—N8A—C9A | 1.5 (2) | C6B—C7B—N8B—C9B | 0.1 (2) |
| O10A—C7A—N8A—C11A | −0.6 (3) | O10B—C7B—N8B—C11B | −2.1 (3) |
| C6A—C7A—N8A—C11A | 178.87 (16) | C6B—C7B—N8B—C11B | 178.37 (16) |
| C7A—N8A—C9A—C12A | 179.28 (17) | C7B—N8B—C9B—C12B | −179.94 (18) |
| C11A—N8A—C9A—C12A | 2.2 (3) | C11B—N8B—C9B—C12B | 1.9 (3) |
| C7A—N8A—C9A—C1A | −1.2 (2) | C7B—N8B—C9B—C1B | −0.5 (2) |
| C11A—N8A—C9A—C1A | −178.31 (17) | C11B—N8B—C9B—C1B | −178.69 (17) |
| C2A—C1A—C9A—C12A | −1.5 (3) | C6B—C1B—C9B—C12B | −179.79 (18) |
| C6A—C1A—C9A—C12A | 179.87 (18) | C2B—C1B—C9B—C12B | −0.2 (4) |
| C2A—C1A—C9A—N8A | 179.0 (2) | C6B—C1B—C9B—N8B | 0.8 (2) |
| C6A—C1A—C9A—N8A | 0.4 (2) | C2B—C1B—C9B—N8B | −179.6 (2) |
| N8A—C9A—C12A—N13A | −7.3 (3) | N8B—C9B—C12B—N13B | 2.2 (3) |
| C1A—C9A—C12A—N13A | 173.28 (18) | C1B—C9B—C12B—N13B | −177.04 (19) |
| N8A—C9A—C12A—C14A | 177.50 (17) | N8B—C9B—C12B—C14B | 179.39 (17) |
| C1A—C9A—C12A—C14A | −1.9 (3) | C1B—C9B—C12B—C14B | 0.1 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N13*A*—H13*A*···N15*B*$^{i}$ | 0.97 | 2.08 | 3.035 (3) | 169 |
| N13*B*—H13*C*···O10*A*$^{ii}$ | 0.94 | 2.04 | 2.948 (2) | 163 |
| N13*B*—H13*D*···N13*A*$^{iii}$ | 0.97 | 2.52 | 3.238 (3) | 131 |

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