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# Crystal structure of 4,4′-dimethoxy-2,2′-bipyridine

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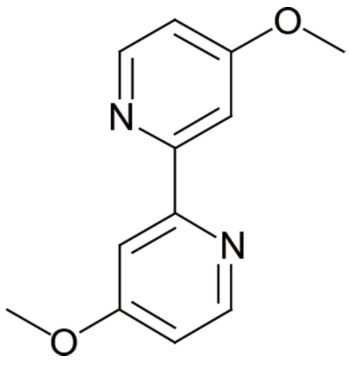
In the title compound, $C_{12}H_{12}N_2O_2$, the dihedral angle between the planes of the two pyridine rings is 5.8 (1)°. Neighbouring molecules are linked *via* C(Me)—H···N interactions, generating a two-dimensional sheet structure; C—H···$\pi$ interactions further link the molecules into a three-dimensional network. An overlapped arrangement of parallel pyridine rings in neighbouring molecules [centroid-to-centroid distance = 3.6655 (15) Å] is observed in the crystal structure.

**Keywords:** crystal structure.

**CCDC reference**: 1414484

## 1. Related literature

For related structure of 4,4′-substituted 2,2′-bipyridines, see: Merritt & Schroeder (1956); Tynan *et al.* (2003); Pearson *et al.* (2004); Haberecht *et al.* (2005); Fujihara *et al.* (2005). For hydrogen-bonded motifs, see: Etter *et al.* (1990); Bernstein *et al.* (1995).




## 2. Experimental

### 2.1. Crystal data

$C_{12}H_{12}N_2O_2$
$M_r$ = 216.24
Monoclinic, $P2_1$
$a$ = 6.4235 (11) Å
$b$ = 10.8139 (18) Å
$c$ = 8.0123 (14) Å
$\beta$ = 109.462 (2)°
$V$ = 524.76 (16) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 200 K
0.24 × 0.07 × 0.05 mm

### 2.2. Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS2014*; Bruker, 2014)
$T_{min}$ = ?, $T_{max}$ = ?
5925 measured reflections
2301 independent reflections
2155 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.084
$S$ = 1.01
2301 reflections
147 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Absolute structure: Flack $x$ determined using 976 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.7 (3)

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

*Cg*1 and *Cg*2 are the centroids of the N1- and N2-rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C11—H11*B*···N1$^{i}$ | 0.98 | 2.58 | 3.503 (3) | 158 |
| C12—H12*B*···N2$^{ii}$ | 0.98 | 2.62 | 3.513 (3) | 151 |
| C1—H1···*Cg*2$^{iii}$ | 0.95 | 2.68 | 3.515 (3) | 146 |
| C12—H12*A*···*Cg*1$^{iv}$ | 0.98 | 2.72 | 3.439 (3) | 134 |

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

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* and *XPREP* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *XCIF* (Bruker, 2014).

Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5860).

## References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2014). *APEX2*, *SADABS*, *SAINT* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Fujihara, T., Suzuki, H. & Nagasawa, A. (2005). *Acta Cryst.* E**61**, o1867–o1868.
Haberecht, M. C., Bolte, M., Bats, J. W., Lerner, H.-W. & Wagner, M. (2005). *Z. Naturforsch. Teil B*, **60**, 745–752.

Merritt, L. L. & Schroeder, E. (1956). *Acta Cryst.* **9**, 801–804.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Pearson, P., Kepert, C. M., Deacon, G. B., Spiccia, L., Warden, A. C., Skelton, B. W. & White, A. H. (2004). *Inorg. Chem.* **43**, 683–691.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Tynan, E., Jensen, P., Kruger, P. E., Lees, A. C. & Nieuwenhuyzen, M. (2003). *Dalton Trans.* pp. 1223–1228.

# supporting information

*Acta Cryst.* (2015). E**71**, o623–o624 [https://doi.org/10.1107/S2056989015013985]

## Crystal structure of 4,4′-dimethoxy-2,2′-bipyridine

**Yukiko Kusano, Keiji Ohno and Takashi Fujihara**

### S1. Comment

The molecular structure of title compound (I) is illustrated in Fig. 1. In the crystal, all bond lengths and angles are similar to those of the other similar 4,4′-substituted 2,2′-bipyridines (Merritt & Schroeder, 1956; Tynan *et al.*, 2003; Pearson *et al.*, 2004; Haberecht *et al.*, 2005; Fujihara *et al.*, 2005). The dihedral angle between two pyridine rings is 5.8 (1)°. The neighbouring molecules are linked *via* intermolecular C–H···N interactions with an $R_2^2(16)$ ring motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995), generating 2D sheet structure as shown in Fig. 2. An overlapped arrangement of parallel pyridine rings in neighbouring molecules [centroid-centroid distance = 3.6655 (15) Å] is observed in the crystal structure. Furthermore, intermolecular C–H···$\pi$ interactions link the molecules into a three-dimensional network, as shown in Fig. 3.

### S2. Synthesis and crystallization

Crystals of (I) suitable for X-ray diffraction were obtained from solutions in acetone of a commercially available sample (Aldrich) by slow evaporation at 298 K. $^1$H NMR (500MHz, $CDCl_3$): $\delta$ 4.10 (s, 6H, -$OCH_3$), 7.03(dd, 2H, py-5H), 8.37(d, 2H, py-H3), 8.56(d, 2H, py-H6).

### S3. Refinement

The H atoms were included in calculated positions and treated as riding atoms: C—H = 0.95-0.98Å with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms and = 1.2$U_{eq}$(C) for aromatic H atoms.

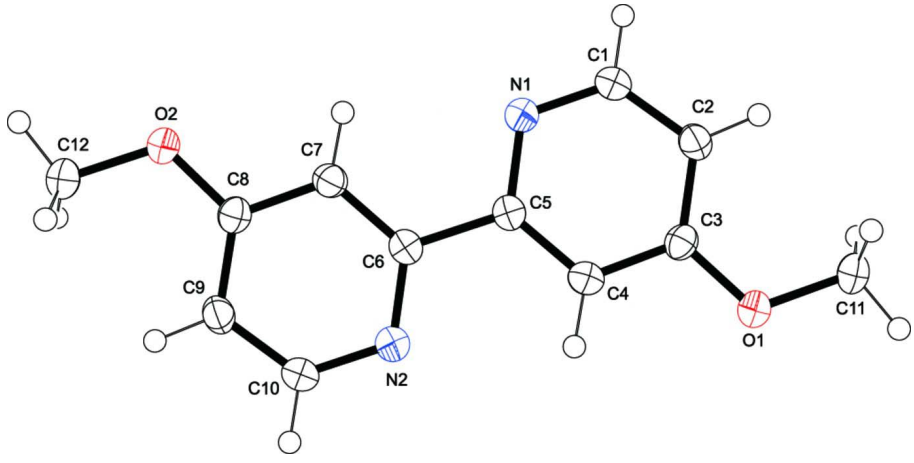



**Figure 1**

The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

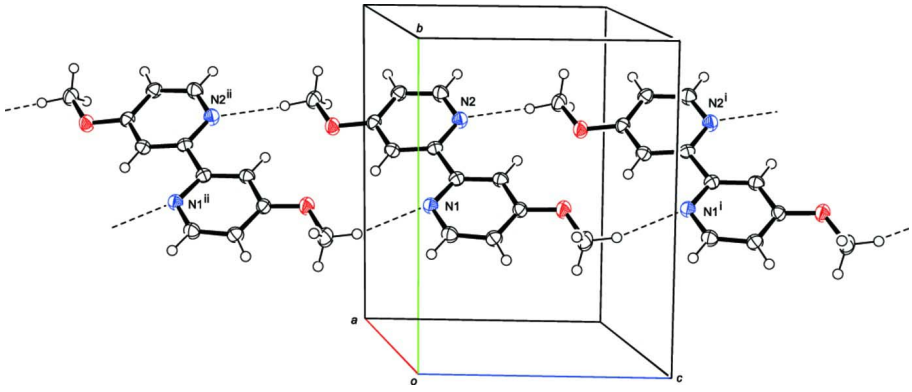



**Figure 2**

Part of the crystal structure of compound (I) showing the formation of 2D sheet. Dashed lines indicate the intermolecular C-H···N interactions. [Symmetry code: (i) *x*, *y*, 1+ *z*; (ii) *x*, *y*, -1+ *z*.]

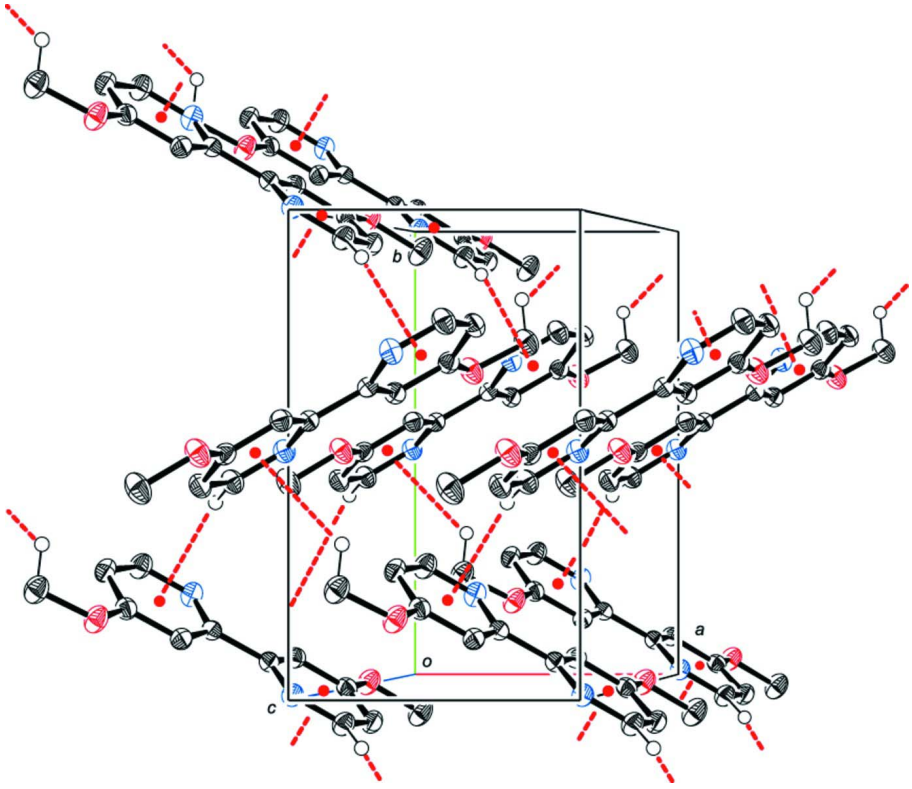



**Figure 3**

Part of the crystal structure showing the intersheet stacking interactions and the weak C-H···$\pi$ hydrogen bonds.

### 4,4′-Dimethoxy-2,2′-bipyridine

*Crystal data*

$C_{12}H_{12}N_2O_2$
$M_r$ = 216.24
Monoclinic, $P2_1$
$a$ = 6.4235 (11) Å
$b$ = 10.8139 (18) Å
$c$ = 8.0123 (14) Å
$\beta$ = 109.462 (2)°
$V$ = 524.76 (16) Å$^3$
$Z$ = 2
$F$(000) = 228

$D_x$ = 1.369 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 3527 reflections
$\theta$ = 2.7–28.3°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 200 K
Plate, colourless
0.24 × 0.07 × 0.05 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: Bruker TXS fine-focus rotating anode
Bruker Helios multilayer confocal mirror monochromator
Detector resolution: 8.333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS2014*; Bruker, 2014)
5925 measured reflections
2301 independent reflections
2155 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014
$\theta_{max}$ = 27.1°, $\theta_{min}$ = 2.7°
$h$ = −8→8
$k$ = −13→13
$l$ = −10→10

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.084
$S$ = 1.01
2301 reflections
147 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.1642P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Absolute structure: Flack $x$ determined using 976 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.7 (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.
Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
- 3.4311 (0.0049) x + 8.4883 (0.0065) y - 0.9456 (0.0066) z = 4.1170 (0.0067)
* -0.0041 (0.0014) N2 * 0.0008 (0.0014) C6 * 0.0044 (0.0014) C7 * -0.0064 (0.0014) C8 * 0.0031 (0.0015) C9 * 0.0021 (0.0016) C10 -0.0086 (0.0030) O2 -0.0684 (0.0042) C12
Rms deviation of fitted atoms = 0.0039
- 3.4675 (0.0048) x + 8.7970 (0.0059) y - 0.1939 (0.0067) z = 4.4232 (0.0036)
Angle to previous plane (with approximate esd) = 5.832 ( 0.127 )
* 0.0007 (0.0014) N1 * 0.0006 (0.0016) C1 * -0.0022 (0.0015) C2 * 0.0024 (0.0015) C3 * -0.0011 (0.0013) C4 * -0.0005 (0.0013) C5 0.0002 (0.0030) O1 -0.0031 (0.0045) C11
Rms deviation of fitted atoms = 0.0015
- 3.4311 (0.0049) x + 8.4883 (0.0065) y - 0.9456 (0.0066) z = 4.1170 (0.0067)
Angle to previous plane (with approximate esd) = 5.832 ( 0.127 )
* -0.0041 (0.0014) N2 * 0.0008 (0.0014) C6 * 0.0044 (0.0014) C7 * -0.0064 (0.0014) C8 * 0.0031 (0.0015) C9 * 0.0021 (0.0016) C10 -3.3185 (0.0031) N1_$4 -3.3333 (0.0027) C1_$4 -3.4592 (0.0024) C2_$4 -3.5727 (0.0026) C3_$4 -3.5648 (0.0032) C4_$4 -3.4354 (0.0034) C5_$4
Rms deviation of fitted atoms = 0.0039
- 3.4675 (0.0048) x + 8.7970 (0.0059) y - 0.1939 (0.0067) z = 4.4232 (0.0036)
Angle to previous plane (with approximate esd) = 5.832 ( 0.127 )
* 0.0007 (0.0014) N1 * 0.0006 (0.0016) C1 * -0.0022 (0.0015) C2 * 0.0024 (0.0015) C3 * -0.0011 (0.0013) C4 * -0.0005 (0.0013) C5 3.5634 (0.0029) N2_$3 3.4535 (0.0033) C6_$3 3.3280 (0.0034) C7_$3 3.3037 (0.0027) C8_$3 3.4295 (0.0025) C9_$3 3.5529 (0.0027) C10_$3
Rms deviation of fitted atoms = 0.0015

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.1486 (3) | 0.4462 (2) | 0.0875 (3) | 0.0267 (5) |
| H1 | −0.2534 | 0.4031 | −0.0068 | 0.032* |
| C2 | −0.1727 (4) | 0.4400 (2) | 0.2528 (3) | 0.0266 (5) |
| H2 | −0.2892 | 0.3940 | 0.2711 | 0.032* |
| C3 | −0.0204 (3) | 0.5037 (2) | 0.3910 (3) | 0.0229 (4) |
| C4 | 0.1487 (3) | 0.56915 (19) | 0.3571 (3) | 0.0236 (4) |
| H4 | 0.2556 | 0.6130 | 0.4492 | 0.028* |
| C5 | 0.1577 (3) | 0.56905 (19) | 0.1864 (3) | 0.0221 (4) |
| C6 | 0.3359 (3) | 0.63676 (19) | 0.1424 (3) | 0.0217 (4) |
| C7 | 0.3547 (4) | 0.6263 (2) | −0.0241 (3) | 0.0238 (4) |
| H7 | 0.2539 | 0.5768 | −0.1126 | 0.029* |
| C8 | 0.5240 (4) | 0.68943 (19) | −0.0599 (3) | 0.0235 (4) |
| C9 | 0.6663 (4) | 0.7627 (2) | 0.0716 (3) | 0.0268 (5) |
| H9 | 0.7823 | 0.8081 | 0.0514 | 0.032* |
| C10 | 0.6319 (4) | 0.7668 (2) | 0.2337 (3) | 0.0295 (5) |
| H10 | 0.7293 | 0.8166 | 0.3239 | 0.035* |
| C11 | −0.1939 (4) | 0.4392 (3) | 0.5974 (3) | 0.0356 (6) |
| H11A | −0.3380 | 0.4719 | 0.5251 | 0.053* |
| H11B | −0.1765 | 0.4482 | 0.7230 | 0.053* |
| H11C | −0.1846 | 0.3515 | 0.5698 | 0.053* |

| | | | | |
|---|---|---|---|---|
| C12 | 0.7110 (4) | 0.7348 (2) | −0.2653 (3) | 0.0321 (5) |
| H12A | 0.7009 | 0.8244 | −0.2509 | 0.048* |
| H12B | 0.7005 | 0.7164 | −0.3876 | 0.048* |
| H12C | 0.8526 | 0.7048 | −0.1844 | 0.048* |
| N1 | 0.0100 (3) | 0.50795 (19) | 0.0503 (2) | 0.0244 (4) |
| N2 | 0.4729 (3) | 0.70612 (19) | 0.2732 (2) | 0.0275 (4) |
| O1 | −0.0221 (3) | 0.50643 (16) | 0.5595 (2) | 0.0307 (4) |
| O2 | 0.5337 (3) | 0.67463 (15) | −0.2257 (2) | 0.0304 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0250 (10) | 0.0285 (11) | 0.0256 (10) | −0.0048 (10) | 0.0069 (8) | −0.0029 (9) |
| C2 | 0.0252 (10) | 0.0274 (11) | 0.0292 (11) | −0.0049 (10) | 0.0118 (9) | −0.0023 (10) |
| C3 | 0.0256 (10) | 0.0222 (10) | 0.0227 (10) | 0.0027 (9) | 0.0105 (8) | 0.0002 (9) |
| C4 | 0.0224 (10) | 0.0225 (10) | 0.0242 (11) | −0.0003 (8) | 0.0055 (8) | −0.0007 (9) |
| C5 | 0.0210 (9) | 0.0208 (10) | 0.0248 (10) | 0.0015 (8) | 0.0082 (8) | 0.0014 (8) |
| C6 | 0.0201 (10) | 0.0196 (10) | 0.0252 (10) | 0.0019 (8) | 0.0071 (8) | 0.0017 (8) |
| C7 | 0.0229 (10) | 0.0234 (10) | 0.0250 (10) | −0.0012 (8) | 0.0077 (8) | −0.0016 (8) |
| C8 | 0.0239 (10) | 0.0239 (11) | 0.0235 (10) | 0.0023 (9) | 0.0090 (8) | 0.0024 (8) |
| C9 | 0.0244 (10) | 0.0279 (11) | 0.0296 (11) | −0.0040 (9) | 0.0112 (9) | 0.0018 (9) |
| C10 | 0.0267 (11) | 0.0338 (13) | 0.0267 (11) | −0.0074 (9) | 0.0071 (9) | −0.0046 (9) |
| C11 | 0.0397 (13) | 0.0443 (14) | 0.0292 (12) | −0.0120 (12) | 0.0200 (10) | −0.0030 (11) |
| C12 | 0.0345 (12) | 0.0370 (13) | 0.0287 (12) | −0.0063 (10) | 0.0158 (10) | 0.0006 (10) |
| N1 | 0.0241 (8) | 0.0265 (9) | 0.0229 (9) | −0.0015 (7) | 0.0081 (7) | −0.0003 (7) |
| N2 | 0.0257 (9) | 0.0321 (10) | 0.0252 (9) | −0.0040 (8) | 0.0091 (7) | −0.0014 (8) |
| O1 | 0.0333 (8) | 0.0362 (9) | 0.0254 (8) | −0.0085 (7) | 0.0137 (6) | −0.0025 (7) |
| O2 | 0.0325 (9) | 0.0366 (9) | 0.0256 (8) | −0.0094 (7) | 0.0144 (7) | −0.0042 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.332 (3) | C8—O2 | 1.359 (3) |
| C1—C2 | 1.385 (3) | C8—C9 | 1.390 (3) |
| C1—H1 | 0.9500 | C9—C10 | 1.389 (3) |
| C2—C3 | 1.391 (3) | C9—H9 | 0.9500 |
| C2—H2 | 0.9500 | C10—N2 | 1.338 (3) |
| C3—O1 | 1.354 (3) | C10—H10 | 0.9500 |
| C3—C4 | 1.398 (3) | C11—O1 | 1.436 (3) |
| C4—C5 | 1.388 (3) | C11—H11A | 0.9800 |
| C4—H4 | 0.9500 | C11—H11B | 0.9800 |
| C5—N1 | 1.355 (3) | C11—H11C | 0.9800 |
| C5—C6 | 1.496 (2) | C12—O2 | 1.436 (3) |
| C6—N2 | 1.349 (3) | C12—H12A | 0.9800 |
| C6—C7 | 1.384 (3) | C12—H12B | 0.9800 |
| C7—C8 | 1.393 (3) | C12—H12C | 0.9800 |
| C7—H7 | 0.9500 | | |
| | | | |
| N1—C1—C2 | 125.1 (2) | C9—C8—C7 | 119.02 (19) |

| | | | |
|---|---|---|---|
| N1—C1—H1 | 117.4 | C10—C9—C8 | 117.2 (2) |
| C2—C1—H1 | 117.4 | C10—C9—H9 | 121.4 |
| C1—C2—C3 | 117.7 (2) | C8—C9—H9 | 121.4 |
| C1—C2—H2 | 121.2 | N2—C10—C9 | 125.3 (2) |
| C3—C2—H2 | 121.2 | N2—C10—H10 | 117.4 |
| O1—C3—C2 | 124.60 (19) | C9—C10—H10 | 117.4 |
| O1—C3—C4 | 116.61 (18) | O1—C11—H11A | 109.5 |
| C2—C3—C4 | 118.79 (19) | O1—C11—H11B | 109.5 |
| C5—C4—C3 | 118.80 (18) | H11A—C11—H11B | 109.5 |
| C5—C4—H4 | 120.6 | O1—C11—H11C | 109.5 |
| C3—C4—H4 | 120.6 | H11A—C11—H11C | 109.5 |
| N1—C5—C4 | 123.02 (19) | H11B—C11—H11C | 109.5 |
| N1—C5—C6 | 115.79 (17) | O2—C12—H12A | 109.5 |
| C4—C5—C6 | 121.18 (17) | O2—C12—H12B | 109.5 |
| N2—C6—C7 | 123.39 (19) | H12A—C12—H12B | 109.5 |
| N2—C6—C5 | 116.19 (17) | O2—C12—H12C | 109.5 |
| C7—C6—C5 | 120.41 (17) | H12A—C12—H12C | 109.5 |
| C6—C7—C8 | 118.92 (19) | H12B—C12—H12C | 109.5 |
| C6—C7—H7 | 120.5 | C1—N1—C5 | 116.58 (18) |
| C8—C7—H7 | 120.5 | C10—N2—C6 | 116.14 (19) |
| O2—C8—C9 | 125.1 (2) | C3—O1—C11 | 117.47 (18) |
| O2—C8—C7 | 115.88 (18) | C8—O2—C12 | 117.40 (17) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | 0.3 (4) | C6—C7—C8—C9 | −1.1 (3) |
| C1—C2—C3—O1 | −180.0 (2) | O2—C8—C9—C10 | −179.9 (2) |
| C1—C2—C3—C4 | −0.5 (3) | C7—C8—C9—C10 | 1.0 (3) |
| O1—C3—C4—C5 | 179.94 (18) | C8—C9—C10—N2 | −0.1 (4) |
| C2—C3—C4—C5 | 0.4 (3) | C2—C1—N1—C5 | −0.1 (3) |
| C3—C4—C5—N1 | −0.2 (3) | C4—C5—N1—C1 | 0.0 (3) |
| C3—C4—C5—C6 | −179.56 (19) | C6—C5—N1—C1 | 179.41 (18) |
| N1—C5—C6—N2 | 174.7 (2) | C9—C10—N2—C6 | −0.5 (4) |
| C4—C5—C6—N2 | −5.8 (3) | C7—C6—N2—C10 | 0.4 (3) |
| N1—C5—C6—C7 | −5.5 (3) | C5—C6—N2—C10 | −179.92 (19) |
| C4—C5—C6—C7 | 173.9 (2) | C2—C3—O1—C11 | −0.2 (3) |
| N2—C6—C7—C8 | 0.4 (3) | C4—C3—O1—C11 | −179.7 (2) |
| C5—C6—C7—C8 | −179.28 (17) | C9—C8—O2—C12 | 3.0 (3) |
| C6—C7—C8—O2 | 179.70 (18) | C7—C8—O2—C12 | −177.8 (2) |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the N1- and N2-rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4···N2 | 0.95 | 2.50 | 2.813 (3) | 99 |
| C7—H7···N1 | 0.95 | 2.46 | 2.789 (3) | 100 |
| C11—H11*B*···N1$^{i}$ | 0.98 | 2.58 | 3.503 (3) | 158 |
| C12—H12*B*···N2$^{ii}$ | 0.98 | 2.62 | 3.513 (3) | 151 |

| | | | | |
|---|---|---|---|---|
| C1—H1···*Cg*2$^{iii}$ | 0.95 | 2.68 | 3.515 (3) | 146 |
| C12—H12*A*···*Cg*1$^{iv}$ | 0.98 | 2.72 | 3.439 (3) | 134 |

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