**organic compounds**

# 4,5-Dimethyl-1,2-diphenyl-1H-imidazole monohydrate

**P. Gayathri,[a] A. Thiruvalluvar,[a]\* K. Saravanan,[b] J. Jayabharathi[b] and R. J. Butcher[c]**

[a]PG Research Department of Physics, Rajah Serfoji Government College (Autonomous), Thanjavur 613 005, Tamilnadu, India, [b]Department of Chemistry, Annamalai University, Annamalai Nagar 608 002, Tamilnadu, India, and [c]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA
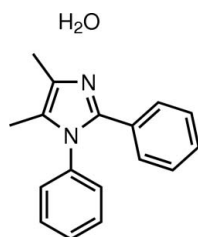
Correspondence e-mail: athiru@vsnl.net

In the title compound, $C_{17}H_{16}N_2 \cdot H_2O$, the imidazole ring is essentially planar [maximum deviation = 0.0037 (7) Å]. The imidazole ring makes dihedral angles of 80.74 (7) and 41.62 (7)° with the phenyl rings attached to the N and C atoms, respectively. The dihedral angle between the two phenyl rings is 75.83 (8)°. Intermolecular O—H···N and O—H···O hydrogen bonds are found in the crystal structure.

## Related literature

For related crystal structures and applications of imidazole derivatives, see: Gayathri et al. (2010a,b).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{17}H_{16}N_2 \cdot H_2O$ | $c = 9.3792$ (1) Å |
| $M_r = 266.33$ | $V = 6122.67$ (9) Å$^3$ |
| Tetragonal, $I4_1/a$ | $Z = 16$ |
| $a = 25.5498$ (2) Å | Cu $K\alpha$ radiation |
| $\mu = 0.57$ mm$^{-1}$ | $0.53 \times 0.42 \times 0.18$ mm |
| $T = 295$ K | |

### Data collection

| | |
|---|---|
| Oxford Diffraction Xcalibur Ruby Gemini diffractometer | 8078 measured reflections |
| Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2010) | 3109 independent reflections |
| | 2610 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.805$, $T_{max} = 1.000$ | $R_{int} = 0.019$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.134$ | |
| $S = 1.08$ | |
| 3109 reflections | $\Delta\rho_{max} = 0.16$ e Å$^{-3}$ |
| 189 parameters | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1W—H1W···N3$^i$ | 0.914 (18) | 2.010 (18) | 2.9111 (14) | 168.6 (16) |
| O1W—H2W···O1W$^i$ | 0.86 (2) | 2.03 (2) | 2.8957 (15) | 175 (2) |

Symmetry code: (i) $y + \frac{1}{4}, -x + \frac{1}{4}, z + \frac{1}{4}$.

Data collection: CrysAlis PRO (Oxford Diffraction, 2010); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SIR2004 (Burla et al., 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: PLATON (Spek, 2009).

## References

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# supporting information

## 4,5-Dimethyl-1,2-diphenyl-1*H*-imidazole monohydrate

### P. Gayathri, A. Thiruvalluvar, K. Saravanan, J. Jayabharathi and R. J. Butcher

### S1. Comment

As part of our research (Gayathri *et al.*, 2010*a*,*b*), we have synthesized the title compound (I) and report its crystal structure here.

In the title compound (Fig. 1), the imidazole ring is essentially planar [maximum deviation of 0.0037 (7) Å for C5]. The imidazole ring makes dihedral angles of 80.74 (7) and 41.62 (7) ° with the phenyl ring (C11—C16) attached to N1 and the phenyl ring (C21—C26) attached to C2, respectively. The dihedral angle between the two phenyl rings is 75.83 (8) °. Intermolecular O1W—H1W···N3 and O1W—H2W···O1W hydrogen bonds are found in the crystal structure (Table 1, Fig. 2).

### S2. Experimental

To pure butane-2,3-dione (1.48 g, 15 mmol), aniline (1.36 g, 15 mmol) and ammonium acetate (1.15 g, 15 mmol) in in ethanol (10 ml) was added benzaldehyde (1.5 g, 15 mmol) over about 1 h with the temperature maintained at 333 K. The reaction mixture was refluxed for 7 days and extracted with dichloromethane. The solid separated was purified by column chromatography using hexane:ethyl acetate as the eluent. Yield: 1.79 g (48%).

### S3. Refinement

H1W and H2W attached to O1W were located in a difference Fourier map and refined freely. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 – 0.96 Å; $U_{iso}$(H) = k$U_{eq}$(C), where k = 1.5 for methyl and 1.2 for all other H atoms. The methyl groups were found to be disordered over two positions. They were each refined as an idealized disordered methyl group.
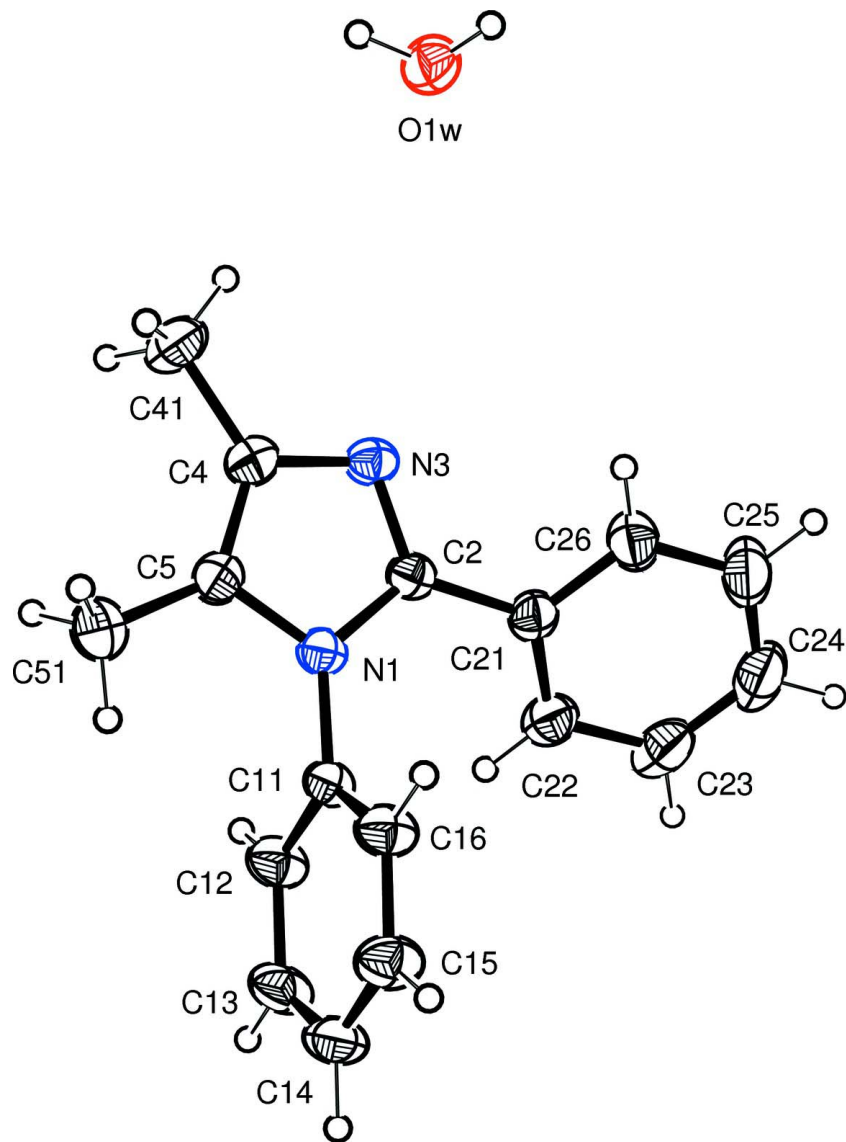
**Figure 1**

The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.

**Figure 2**

The packing of the title compound, viewed down the $c$ axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

**4,5-Dimethyl-1,2-diphenyl-1H-imidazole monohydrate**

*Crystal data*

| | |
|---|---|
| $C_{17}H_{16}N_2 \cdot H_2O$ | $D_x = 1.156$ Mg m$^{-3}$ |
| $M_r = 266.33$ | Melting point: 375 K |
| Tetragonal, $I4_1/a$ | Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å |
| Hall symbol: -I 4ad | Cell parameters from 4027 reflections |
| $a = 25.5498$ (2) Å | $\theta = 4.9$–77.4° |
| $c = 9.3792$ (1) Å | $\mu = 0.57$ mm$^{-1}$ |
| $V = 6122.67$ (9) Å$^3$ | $T = 295$ K |
| $Z = 16$ | Irregular plate, colourless |
| $F(000) = 2272$ | $0.53 \times 0.42 \times 0.18$ mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Ruby Gemini diffractometer | $\omega$ scans |
| | Absorption correction: multi-scan |
| Radiation source: Enhance (Cu) X-ray Source | (*CrysAlis PRO*; Oxford Diffraction, 2010) |
| Graphite monochromator | $T_{min} = 0.805$, $T_{max} = 1.000$ |
| Detector resolution: 10.5081 pixels mm$^{-1}$ | 8078 measured reflections |

3109 independent reflections
2610 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 77.6°$, $\theta_{min} = 4.9°$

$h = -29 \rightarrow 31$
$k = -31 \rightarrow 31$
$l = -6 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.134$
$S = 1.08$
3109 reflections
189 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0876P)^2 + 0.4988P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 $F^2 > 2\sigma(F^2)$ 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* | $U_{iso}*/U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| N1 | 0.00564 (4) | 0.01347 (4) | 0.24242 (9) | 0.0428 (3) | |
| N3 | 0.09186 (4) | 0.00845 (4) | 0.23202 (10) | 0.0452 (3) | |
| C2 | 0.04817 (4) | −0.01899 (5) | 0.23981 (11) | 0.0412 (3) | |
| C4 | 0.07726 (5) | 0.06023 (5) | 0.22951 (13) | 0.0487 (3) | |
| C5 | 0.02420 (5) | 0.06453 (5) | 0.23682 (13) | 0.0488 (3) | |
| C11 | −0.04871 (4) | −0.00047 (5) | 0.25460 (11) | 0.0421 (3) | |
| C12 | −0.07965 (5) | −0.00048 (6) | 0.13375 (13) | 0.0582 (5) | |
| C13 | −0.13211 (5) | −0.01271 (7) | 0.14490 (16) | 0.0649 (5) | |
| C14 | −0.15362 (5) | −0.02441 (7) | 0.27589 (17) | 0.0618 (4) | |
| C15 | −0.12261 (5) | −0.02413 (7) | 0.39614 (15) | 0.0627 (5) | |
| C16 | −0.06994 (5) | −0.01241 (6) | 0.38579 (12) | 0.0526 (4) | |
| C21 | 0.04616 (5) | −0.07654 (5) | 0.24358 (12) | 0.0473 (3) | |
| C22 | 0.01046 (6) | −0.10535 (6) | 0.16451 (16) | 0.0597 (4) | |
| C23 | 0.01189 (7) | −0.15977 (6) | 0.1680 (2) | 0.0778 (6) | |
| C24 | 0.04837 (8) | −0.18527 (7) | 0.2490 (2) | 0.0856 (7) | |
| C25 | 0.08410 (8) | −0.15716 (7) | 0.3262 (2) | 0.0869 (7) | |
| C26 | 0.08325 (6) | −0.10288 (6) | 0.32454 (17) | 0.0662 (5) | |
| C41 | 0.11729 (7) | 0.10273 (6) | 0.2167 (2) | 0.0696 (5) | |
| C51 | −0.01126 (7) | 0.11082 (6) | 0.2437 (2) | 0.0704 (5) | |
| O1W | 0.24177 (4) | 0.04630 (4) | 0.44390 (11) | 0.0590 (3) | |
| H12 | −0.06522 | 0.00770 | 0.04549 | 0.0699* | |

| | | | | | |
|------|----------|----------|-----------|-----------|-------|
| H13 | −0.15303 | −0.01307 | 0.06375 | 0.0779* | |
| H14 | −0.18902 | −0.03247 | 0.28311 | 0.0742* | |
| H15 | −0.13718 | −0.03186 | 0.48453 | 0.0753* | |
| H16 | −0.04894 | −0.01257 | 0.46680 | 0.0631* | |
| H22 | −0.01446 | −0.08828 | 0.10917 | 0.0716* | |
| H23 | −0.01212 | −0.17894 | 0.11479 | 0.0933* | |
| H24 | 0.04891 | −0.22165 | 0.25155 | 0.1027* | |
| H25 | 0.10914 | −0.17460 | 0.38022 | 0.1043* | |
| H26 | 0.10756 | −0.08410 | 0.37773 | 0.0794* | |
| H41A | 0.15164 | 0.08752 | 0.21390 | 0.1045* | 0.500 |
| H41B | 0.11467 | 0.12573 | 0.29733 | 0.1045* | 0.500 |
| H41C | 0.11126 | 0.12219 | 0.13073 | 0.1045* | 0.500 |
| H41D | 0.10007 | 0.13611 | 0.21408 | 0.1045* | 0.500 |
| H41E | 0.13704 | 0.09790 | 0.13064 | 0.1045* | 0.500 |
| H41F | 0.14045 | 0.10144 | 0.29724 | 0.1045* | 0.500 |
| H51A | −0.04695 | 0.09918 | 0.24795 | 0.1055* | 0.500 |
| H51B | −0.00634 | 0.13205 | 0.16032 | 0.1055* | 0.500 |
| H51C | −0.00332 | 0.13102 | 0.32724 | 0.1055* | 0.500 |
| H51D | 0.00921 | 0.14232 | 0.24239 | 0.1055* | 0.500 |
| H51E | −0.03140 | 0.10945 | 0.33002 | 0.1055* | 0.500 |
| H51F | −0.03442 | 0.11048 | 0.16310 | 0.1055* | 0.500 |
| H1W | 0.2423 (7) | 0.0816 (7) | 0.4596 (18) | 0.064 (4)* | |
| H2W | 0.2563 (9) | 0.0340 (9) | 0.520 (2) | 0.095 (7)* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|------------|------------|-------------|-------------|-------------|-------------|
| N1 | 0.0387 (5) | 0.0480 (5) | 0.0416 (5) | −0.0005 (4) | −0.0003 (3) | 0.0024 (4) |
| N3 | 0.0396 (5) | 0.0533 (5) | 0.0427 (4) | −0.0041 (4) | 0.0026 (4) | 0.0011 (4) |
| C2 | 0.0382 (5) | 0.0498 (6) | 0.0357 (5) | −0.0006 (4) | 0.0019 (4) | 0.0033 (4) |
| C4 | 0.0484 (6) | 0.0510 (6) | 0.0468 (6) | −0.0068 (5) | 0.0022 (5) | −0.0010 (5) |
| C5 | 0.0512 (6) | 0.0466 (6) | 0.0485 (6) | −0.0023 (5) | −0.0005 (5) | 0.0010 (5) |
| C11 | 0.0363 (5) | 0.0498 (6) | 0.0403 (5) | 0.0019 (4) | −0.0005 (4) | 0.0015 (4) |
| C12 | 0.0493 (7) | 0.0851 (10) | 0.0402 (6) | −0.0004 (6) | −0.0044 (5) | 0.0102 (6) |
| C13 | 0.0463 (7) | 0.0911 (10) | 0.0574 (7) | 0.0015 (6) | −0.0156 (6) | 0.0082 (7) |
| C14 | 0.0370 (6) | 0.0771 (9) | 0.0713 (8) | −0.0010 (5) | −0.0022 (6) | 0.0031 (7) |
| C15 | 0.0496 (7) | 0.0881 (10) | 0.0505 (7) | −0.0062 (6) | 0.0081 (5) | 0.0060 (7) |
| C16 | 0.0457 (6) | 0.0745 (8) | 0.0377 (5) | −0.0039 (5) | −0.0026 (4) | 0.0032 (5) |
| C21 | 0.0448 (6) | 0.0486 (6) | 0.0486 (6) | 0.0008 (4) | 0.0111 (5) | 0.0060 (5) |
| C22 | 0.0538 (7) | 0.0548 (7) | 0.0705 (8) | −0.0052 (5) | 0.0082 (6) | −0.0030 (6) |
| C23 | 0.0768 (10) | 0.0573 (8) | 0.0992 (12) | −0.0150 (7) | 0.0224 (9) | −0.0099 (8) |
| C24 | 0.0900 (12) | 0.0491 (8) | 0.1177 (15) | 0.0020 (8) | 0.0344 (11) | 0.0162 (9) |
| C25 | 0.0846 (12) | 0.0666 (10) | 0.1096 (14) | 0.0172 (9) | 0.0127 (11) | 0.0349 (10) |
| C26 | 0.0621 (8) | 0.0636 (8) | 0.0729 (9) | 0.0066 (6) | 0.0011 (7) | 0.0178 (7) |
| C41 | 0.0635 (8) | 0.0572 (8) | 0.0882 (10) | −0.0169 (6) | 0.0119 (8) | −0.0054 (7) |
| C51 | 0.0643 (9) | 0.0542 (8) | 0.0926 (11) | 0.0080 (6) | −0.0007 (8) | −0.0011 (7) |
| O1W | 0.0640 (5) | 0.0518 (6) | 0.0611 (5) | −0.0050 (4) | −0.0054 (4) | −0.0043 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1W—H2W | 0.86 (2) | C12—H12 | 0.9300 |
| O1W—H1W | 0.914 (18) | C13—H13 | 0.9300 |
| N1—C5 | 1.3891 (16) | C14—H14 | 0.9300 |
| N1—C2 | 1.3672 (15) | C15—H15 | 0.9300 |
| N1—C11 | 1.4381 (15) | C16—H16 | 0.9300 |
| N3—C4 | 1.3748 (16) | C22—H22 | 0.9300 |
| N3—C2 | 1.3202 (15) | C23—H23 | 0.9300 |
| C2—C21 | 1.4717 (18) | C24—H24 | 0.9300 |
| C4—C41 | 1.497 (2) | C25—H25 | 0.9300 |
| C4—C5 | 1.3618 (18) | C26—H26 | 0.9300 |
| C5—C51 | 1.491 (2) | C41—H41B | 0.9600 |
| C11—C12 | 1.3819 (16) | C41—H41A | 0.9600 |
| C11—C16 | 1.3789 (16) | C41—H41E | 0.9600 |
| C12—C13 | 1.3803 (18) | C41—H41C | 0.9600 |
| C13—C14 | 1.379 (2) | C41—H41D | 0.9600 |
| C14—C15 | 1.378 (2) | C41—H41F | 0.9600 |
| C15—C16 | 1.3820 (18) | C51—H51B | 0.9600 |
| C21—C26 | 1.388 (2) | C51—H51C | 0.9600 |
| C21—C22 | 1.387 (2) | C51—H51E | 0.9600 |
| C22—C23 | 1.391 (2) | C51—H51F | 0.9600 |
| C23—C24 | 1.368 (3) | C51—H51D | 0.9600 |
| C24—C25 | 1.369 (3) | C51—H51A | 0.9600 |
| C25—C26 | 1.387 (2) | | |
| | | | |
| O1W⋯O1W[i] | 2.8957 (15) | C41⋯H51D | 2.9500 |
| O1W⋯O1W[ii] | 2.8957 (15) | C51⋯H41D | 2.9300 |
| O1W⋯N3[ii] | 2.9111 (14) | H1W⋯N3[ii] | 2.010 (18) |
| O1W⋯H14[iii] | 2.8200 | H1W⋯H41A[ii] | 2.4700 |
| O1W⋯H2W[i] | 2.03 (2) | H1W⋯C4[ii] | 2.910 (18) |
| O1W⋯H13[iv] | 2.7900 | H1W⋯C2[ii] | 3.098 (18) |
| O1W⋯H15[v] | 2.7800 | H2W⋯O1W[ii] | 2.03 (2) |
| O1W⋯H41A[ii] | 2.7900 | H2W⋯H14[v] | 2.5200 |
| O1W⋯H14[v] | 2.9100 | H12⋯N3[vi] | 2.7200 |
| N3⋯O1W[i] | 2.9111 (14) | H12⋯C2[vi] | 2.7300 |
| N1⋯H16[v] | 2.9400 | H13⋯O1W[viii] | 2.7900 |
| N1⋯H22 | 2.9300 | H14⋯O1W[vii] | 2.8200 |
| N3⋯H26 | 2.7600 | H14⋯O1W[v] | 2.9100 |
| N3⋯H1W[i] | 2.010 (18) | H14⋯H2W[v] | 2.5200 |
| N3⋯H12[vi] | 2.7200 | H15⋯O1W[v] | 2.7800 |
| C11⋯C22 | 3.191 (2) | H16⋯C2[v] | 2.8700 |
| C12⋯C22 | 3.544 (2) | H16⋯N1[v] | 2.9400 |
| C12⋯C51 | 3.493 (2) | H22⋯N1 | 2.9300 |
| C22⋯C12 | 3.544 (2) | H22⋯C11 | 2.7700 |
| C22⋯C11 | 3.191 (2) | H22⋯C12 | 2.8000 |
| C23⋯C25[vii] | 3.597 (3) | H24⋯C24[iii] | 3.0800 |
| C25⋯C23[iii] | 3.597 (3) | H24⋯H51C[i] | 2.5600 |

| | | | |
|---|---|---|---|
| C51···C12 | 3.493 (2) | H25···C23ⁱⁱⁱ | 2.9600 |
| C2···H1Wⁱ | 3.098 (18) | H25···C22ⁱⁱⁱ | 3.0600 |
| C2···H16ᵛ | 2.8700 | H26···N3 | 2.7600 |
| C2···H12ᵛⁱ | 2.7300 | H41A···H1Wⁱ | 2.4700 |
| C4···H1Wⁱ | 2.910 (18) | H41A···O1Wⁱ | 2.7900 |
| C11···H22 | 2.7700 | H41B···C24ⁱⁱ | 2.9900 |
| C11···H51A | 2.5500 | H41B···C25ⁱⁱ | 2.8600 |
| C11···H51E | 2.9300 | H41B···C26ⁱⁱ | 2.9200 |
| C11···H51F | 2.9800 | H41D···C51 | 2.9300 |
| C12···H51F | 3.0700 | H41D···H51D | 2.3400 |
| C12···H22 | 2.8000 | H41F···C26ⁱⁱ | 3.0900 |
| C12···H51A | 2.8900 | H51A···C11 | 2.5500 |
| C22···H25ᵛⁱⁱ | 3.0600 | H51A···C12 | 2.8900 |
| C23···H25ᵛⁱⁱ | 2.9600 | H51C···C24ⁱⁱ | 2.9800 |
| C24···H51Cⁱ | 2.9800 | H51C···H24ⁱⁱ | 2.5600 |
| C24···H41Bⁱ | 2.9900 | H51D···C41 | 2.9500 |
| C24···H24ᵛⁱⁱ | 3.0800 | H51D···H41D | 2.3400 |
| C25···H41Bⁱ | 2.8600 | H51E···C11 | 2.9300 |
| C26···H41Fⁱ | 3.0900 | H51F···C11 | 2.9800 |
| C26···H41Bⁱ | 2.9200 | H51F···C12 | 3.0700 |
| | | | |
| H1W—O1W—H2W | 102.7 (18) | C26—C25—H25 | 120.00 |
| C2—N1—C11 | 128.22 (10) | C24—C25—H25 | 120.00 |
| C5—N1—C11 | 124.42 (10) | C25—C26—H26 | 120.00 |
| C2—N1—C5 | 107.32 (10) | C21—C26—H26 | 120.00 |
| C2—N3—C4 | 106.41 (10) | C4—C41—H41A | 109.00 |
| N1—C2—N3 | 110.54 (11) | C4—C41—H41C | 109.00 |
| N1—C2—C21 | 125.30 (10) | C4—C41—H41D | 109.00 |
| N3—C2—C21 | 124.15 (10) | C4—C41—H41B | 109.00 |
| N3—C4—C41 | 120.94 (12) | C4—C41—H41F | 109.00 |
| C5—C4—C41 | 128.74 (12) | H41A—C41—H41B | 109.00 |
| N3—C4—C5 | 110.30 (11) | H41A—C41—H41C | 109.00 |
| N1—C5—C51 | 122.40 (12) | H41A—C41—H41D | 141.00 |
| C4—C5—C51 | 132.14 (13) | H41A—C41—H41E | 56.00 |
| N1—C5—C4 | 105.43 (11) | H41A—C41—H41F | 56.00 |
| N1—C11—C16 | 120.37 (10) | C4—C41—H41E | 109.00 |
| C12—C11—C16 | 120.46 (11) | H41B—C41—H41D | 56.00 |
| N1—C11—C12 | 119.16 (10) | H41B—C41—H41E | 141.00 |
| C11—C12—C13 | 119.56 (12) | H41B—C41—H41F | 56.00 |
| C12—C13—C14 | 120.25 (13) | H41C—C41—H41D | 56.00 |
| C13—C14—C15 | 119.93 (12) | H41C—C41—H41E | 56.00 |
| C14—C15—C16 | 120.22 (13) | H41C—C41—H41F | 141.00 |
| C11—C16—C15 | 119.58 (11) | H41D—C41—H41E | 109.00 |
| C2—C21—C26 | 118.27 (11) | H41D—C41—H41F | 109.00 |
| C22—C21—C26 | 118.95 (13) | H41E—C41—H41F | 109.00 |
| C2—C21—C22 | 122.71 (11) | H41B—C41—H41C | 109.00 |
| C21—C22—C23 | 120.04 (14) | C5—C51—H51B | 109.00 |
| C22—C23—C24 | 120.47 (16) | C5—C51—H51C | 109.00 |

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| C23—C24—C25 | 119.90 (17) | C5—C51—H51A | 109.00 |
| C24—C25—C26 | 120.55 (17) | C5—C51—H51E | 109.00 |
| C21—C26—C25 | 120.10 (15) | C5—C51—H51F | 109.00 |
| C13—C12—H12 | 120.00 | C5—C51—H51D | 109.00 |
| C11—C12—H12 | 120.00 | H51A—C51—H51C | 109.00 |
| C14—C13—H13 | 120.00 | H51A—C51—H51D | 141.00 |
| C12—C13—H13 | 120.00 | H51A—C51—H51E | 56.00 |
| C13—C14—H14 | 120.00 | H51A—C51—H51F | 56.00 |
| C15—C14—H14 | 120.00 | H51B—C51—H51C | 109.00 |
| C16—C15—H15 | 120.00 | H51B—C51—H51D | 56.00 |
| C14—C15—H15 | 120.00 | H51B—C51—H51E | 141.00 |
| C11—C16—H16 | 120.00 | H51B—C51—H51F | 56.00 |
| C15—C16—H16 | 120.00 | H51C—C51—H51D | 56.00 |
| C23—C22—H22 | 120.00 | H51C—C51—H51E | 56.00 |
| C21—C22—H22 | 120.00 | H51C—C51—H51F | 141.00 |
| C22—C23—H23 | 120.00 | H51D—C51—H51E | 109.00 |
| C24—C23—H23 | 120.00 | H51D—C51—H51F | 109.00 |
| C23—C24—H24 | 120.00 | H51E—C51—H51F | 109.00 |
| C25—C24—H24 | 120.00 | H51A—C51—H51B | 109.00 |
| | | | |
| C5—N1—C2—N3 | −0.41 (12) | N3—C4—C5—N1 | −0.66 (13) |
| C5—N1—C2—C21 | −179.82 (10) | N3—C4—C5—C51 | 177.15 (14) |
| C11—N1—C2—N3 | −178.01 (9) | C41—C4—C5—N1 | 177.86 (13) |
| C11—N1—C2—C21 | 2.58 (17) | C41—C4—C5—C51 | −4.3 (2) |
| C2—N1—C5—C4 | 0.65 (12) | N1—C11—C12—C13 | −178.61 (13) |
| C2—N1—C5—C51 | −177.43 (12) | C16—C11—C12—C13 | −0.2 (2) |
| C11—N1—C5—C4 | 178.36 (10) | N1—C11—C16—C15 | 177.99 (13) |
| C11—N1—C5—C51 | 0.28 (18) | C12—C11—C16—C15 | −0.4 (2) |
| C2—N1—C11—C12 | −101.64 (14) | C11—C12—C13—C14 | 0.6 (2) |
| C2—N1—C11—C16 | 79.95 (16) | C12—C13—C14—C15 | −0.3 (3) |
| C5—N1—C11—C12 | 81.14 (15) | C13—C14—C15—C16 | −0.3 (3) |
| C5—N1—C11—C16 | −97.27 (15) | C14—C15—C16—C11 | 0.7 (2) |
| C4—N3—C2—N1 | 0.00 (13) | C2—C21—C22—C23 | 177.34 (13) |
| C4—N3—C2—C21 | 179.42 (10) | C26—C21—C22—C23 | 0.5 (2) |
| C2—N3—C4—C5 | 0.42 (13) | C2—C21—C26—C25 | −177.29 (14) |
| C2—N3—C4—C41 | −178.24 (12) | C22—C21—C26—C25 | −0.3 (2) |
| N1—C2—C21—C22 | 42.85 (17) | C21—C22—C23—C24 | 0.0 (3) |
| N1—C2—C21—C26 | −140.30 (12) | C22—C23—C24—C25 | −0.6 (3) |
| N3—C2—C21—C22 | −136.48 (13) | C23—C24—C25—C26 | 0.8 (3) |
| N3—C2—C21—C26 | 40.36 (17) | C24—C25—C26—C21 | −0.4 (3) |

Symmetry codes: (i) −*y*+1/4, *x*−1/4, *z*−1/4; (ii) *y*+1/4, −*x*+1/4, *z*+1/4; (iii) *y*+1/4, −*x*−1/4, −*z*+3/4; (iv) −*y*+1/4, *x*+1/4, −*z*+1/4; (v) −*x*, −*y*, −*z*+1; (vi) −*x*, −*y*, −*z*; (vii) −*y*−1/4, *x*−1/4, −*z*+3/4; (viii) *y*−1/4, −*x*+1/4, −*z*+1/4.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*W*···N3[ii] | 0.914 (18) | 2.010 (18) | 2.9111 (14) | 168.6 (16) |

| O1$W$—H2$W$···O1$W$[ii] | 0.86 (2) | 2.03 (2) | 2.8957 (15) | 175 (2) |

Symmetry code: (ii) $y+1/4, -x+1/4, z+1/4$.