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# 2-Diethylamino-6-methylpyrimidin-4(3*H*)-one

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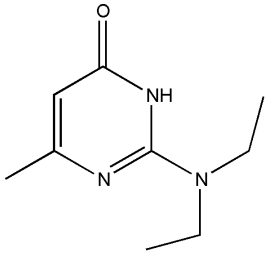
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.002 Å; some non-H atoms missing; $R$ factor = 0.045; $wR$ factor = 0.097; data-to-parameter ratio = 19.3.

The title compound, $C_9H_{15}N_3O$, contains four molecules (*A*, *B*, *C* and *D*) in the asymmetric unit. In the crystal, the *A*+*A* and *D*+*D* pairs form inversion dimers linked by pairs of N—H···O hydrogen bonds. The *B*+*C* pairing is linked by the same bonds. The dimers are further linked by weak C—H···O interactions.

## Related literature

For further details of the synthesis, see: Huang *et al.* (2007). For the biological activity of related compounds, see, for example: Atul *et al.* (2010); Liu, Jian & Tan (2011); Liu, Jian, Tan *et al.* (2011).




## Experimental

### *Crystal data*

$C_9H_{15}N_3O$
$M_r$ = 181.24
Triclinic, $P\overline{1}$
$a$ = 11.799 (5) Å
$b$ = 12.136 (5) Å
$c$ = 15.023 (5) Å
$\alpha$ = 92.753 (5)°
$\beta$ = 94.538 (6)°
$\gamma$ = 112.103 (5)°
$V$ = 1979.6 (13) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 113 K
0.20 × 0.18 × 0.10 mm

### *Data collection*

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.984, $T_{max}$ = 0.992
20802 measured reflections
9288 independent reflections
6322 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.097
$S$ = 0.96
9288 reflections
481 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O1$^{i}$ | 0.88 | 2.02 | 2.8420 (19) | 156 |
| N4—H4*A*···O3 | 0.88 | 1.98 | 2.8407 (18) | 164 |
| N8—H8*C*···O2 | 0.88 | 1.99 | 2.8420 (18) | 162 |
| N10—H10*A*···O4$^{ii}$ | 0.88 | 1.98 | 2.8248 (18) | 162 |
| C6—H6*A*···O1$^{i}$ | 0.99 | 2.22 | 3.116 (2) | 150 |
| C15—H15*A*···O3 | 0.99 | 2.35 | 3.120 (2) | 134 |
| C16—H16*B*···O1 | 0.98 | 2.58 | 3.507 (2) | 158 |
| C26—H26*A*···O2 | 0.99 | 2.31 | 3.130 (2) | 139 |
| C33—H33*A*···O4$^{ii}$ | 0.99 | 2.42 | 3.143 (2) | 130 |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y, -z$.

Data collection: *CrystalClear* (Rigaku/MSC, 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: *CrystalStructure* (Rigaku/MSC, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6420).

## References

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o2904 [ **doi:10.1107/S1600536811040451** ]

# 2-Diethylamino-6-methylpyrimidin-4(3*H*)-one

**M.-Y. Wang**

## Experimental

1,1-Diethylguanidine and ethyl 3-oxobutanoate was stirred in EtOH/NaOH solution. The mixture was refluxed for 1 h. The product was collected. Colourless prisms were obtained from EtOH soltion.

## Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

## Figures

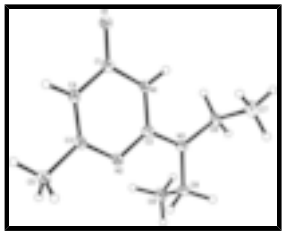

Fig. 1. The structure of one of the moleucles of (I) showing 30% displacement ellipsoids.

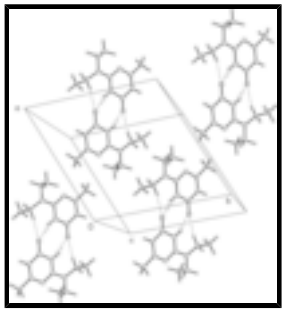

Fig. 2. The crystal packing for (I).

## 2-Diethylamino-6-methylpyrimidin-4(3*H*)-one

*Crystal data*

| | |
|---|---|
| $C_9H_{15}N_3O$ | $Z$ = 8 |
| $M_r$ = 181.24 | $F$(000) = 784 |
| Triclinic, $P\overline{1}$ | $D_x$ = 1.216 Mg m$^{-3}$ |
| $a$ = 11.799 (5) Å | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| $b$ = 12.136 (5) Å | Cell parameters from 6611 reflections |
| $c$ = 15.023 (5) Å | θ = 1.8–27.9° |
| α = 92.753 (5)° | μ = 0.08 mm$^{-1}$ |

| | |
|---|---|
| β = 94.538 (6)° | $T$ = 113 K |
| γ = 112.103 (5)° | Prism, colorless |
| $V$ = 1979.6 (13) Å$^3$ | 0.20 × 0.18 × 0.10 mm |

*Data collection*

| | |
|---|---|
| Rigaku Saturn CCD area-detector diffractometer | 9288 independent reflections |
| Radiation source: rotating anode | 6322 reflections with $I > 2\sigma(I)$ |
| multilayer | $R_{int}$ = 0.033 |
| Detector resolution: 14.63 pixels mm$^{-1}$ | $\theta_{max}$ = 27.9°, $\theta_{min}$ = 1.8° |
| ω and φ scans | $h$ = −15→15 |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005) | $k$ = −15→15 |
| $T_{min}$ = 0.984, $T_{max}$ = 0.992 | $l$ = −14→19 |
| 20802 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.097 | H-atom parameters constrained |
| $S$ = 0.96 | $w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 9288 reflections | $(\Delta/\sigma)_{max}$ = 0.001 |
| 481 parameters | $\Delta\rho_{max}$ = 0.19 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.20 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.99183 (8) | 0.40717 (8) | 0.41209 (6) | 0.0251 (2) |
| O2 | 0.72491 (9) | 0.84710 (8) | 0.18851 (6) | 0.0301 (2) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.75913 (8) | 0.63637 (8) | 0.30675 (6) | 0.0274 (2) |
| O4 | 0.49910 (8) | 0.07510 (8) | 0.09424 (6) | 0.0274 (2) |
| N1 | 0.82458 (10) | 0.39755 (9) | 0.48181 (7) | 0.0194 (2) |
| H1A | 0.8668 | 0.4686 | 0.5096 | 0.023* |
| N2 | 0.63604 (10) | 0.23127 (9) | 0.45981 (7) | 0.0232 (3) |
| N3 | 0.65972 (10) | 0.38934 (9) | 0.56118 (7) | 0.0231 (3) |
| N4 | 0.89914 (10) | 0.87803 (9) | 0.27973 (7) | 0.0203 (3) |
| H4A | 0.8694 | 0.8027 | 0.2916 | 0.024* |
| N5 | 1.06587 (10) | 1.06548 (9) | 0.30369 (7) | 0.0203 (3) |
| N6 | 1.07319 (10) | 0.90590 (9) | 0.37854 (7) | 0.0224 (3) |
| N7 | 0.41150 (10) | 0.42370 (9) | 0.20112 (7) | 0.0215 (3) |
| N8 | 0.58723 (9) | 0.60348 (9) | 0.21177 (7) | 0.0205 (3) |
| H8C | 0.6222 | 0.6746 | 0.1925 | 0.025* |
| N9 | 0.41080 (10) | 0.57771 (9) | 0.11655 (7) | 0.0223 (3) |
| N10 | 0.67058 (9) | 0.11616 (9) | 0.02141 (7) | 0.0191 (2) |
| H10A | 0.6319 | 0.0523 | −0.0159 | 0.023* |
| N11 | 0.85329 (10) | 0.28537 (9) | 0.06299 (7) | 0.0208 (3) |
| N12 | 0.84578 (10) | 0.15135 (9) | −0.05414 (7) | 0.0238 (3) |
| C1 | 0.88085 (12) | 0.35068 (11) | 0.42104 (8) | 0.0206 (3) |
| C2 | 0.70603 (12) | 0.33780 (11) | 0.50029 (9) | 0.0207 (3) |
| C3 | 0.68696 (12) | 0.18461 (11) | 0.39732 (9) | 0.0233 (3) |
| C4 | 0.80429 (12) | 0.23978 (11) | 0.37574 (9) | 0.0230 (3) |
| H4 | 0.8342 | 0.2037 | 0.3305 | 0.028* |
| C5 | 0.60347 (13) | 0.06516 (12) | 0.35259 (10) | 0.0342 (4) |
| H5A | 0.5395 | 0.0749 | 0.3117 | 0.051* |
| H5B | 0.5650 | 0.0121 | 0.3982 | 0.051* |
| H5C | 0.6513 | 0.0304 | 0.3187 | 0.051* |
| C6 | 0.72752 (12) | 0.50937 (11) | 0.60599 (9) | 0.0239 (3) |
| H6A | 0.8147 | 0.5207 | 0.6206 | 0.029* |
| H6B | 0.6929 | 0.5165 | 0.6629 | 0.029* |
| C7 | 0.72098 (14) | 0.60672 (12) | 0.54788 (10) | 0.0361 (4) |
| H7A | 0.7538 | 0.5991 | 0.4910 | 0.054* |
| H7B | 0.7698 | 0.6852 | 0.5792 | 0.054* |
| H7C | 0.6352 | 0.5986 | 0.5361 | 0.054* |
| C8 | 0.53807 (12) | 0.32129 (12) | 0.58906 (9) | 0.0287 (3) |
| H8A | 0.4851 | 0.2675 | 0.5377 | 0.034* |
| H8B | 0.4992 | 0.3770 | 0.6075 | 0.034* |
| C9 | 0.54776 (14) | 0.24807 (12) | 0.66640 (9) | 0.0342 (4) |
| H9A | 0.5819 | 0.1898 | 0.6471 | 0.051* |
| H9B | 0.4658 | 0.2061 | 0.6852 | 0.051* |
| H9C | 0.6018 | 0.3011 | 0.7167 | 0.051* |
| C10 | 0.82874 (12) | 0.91843 (12) | 0.22073 (9) | 0.0217 (3) |
| C11 | 1.01310 (12) | 0.95142 (11) | 0.32001 (8) | 0.0194 (3) |
| C12 | 1.00049 (12) | 1.10774 (11) | 0.24514 (8) | 0.0206 (3) |
| C13 | 0.88573 (12) | 1.03962 (11) | 0.20382 (9) | 0.0224 (3) |
| H13 | 0.8444 | 1.0739 | 0.1638 | 0.027* |
| C14 | 1.06188 (12) | 1.23722 (11) | 0.23059 (9) | 0.0251 (3) |
| H14A | 1.0148 | 1.2570 | 0.1816 | 0.038* |
| H14B | 1.1455 | 1.2535 | 0.2151 | 0.038* |

| | | | | |
|---|---|---|---|---|
| H14C | 1.0655 | 1.2859 | 0.2855 | 0.038* |
| C15 | 1.01969 (12) | 0.78372 (11) | 0.40542 (9) | 0.0240 (3) |
| H15A | 0.9296 | 0.7599 | 0.4048 | 0.029* |
| H15B | 1.0534 | 0.7821 | 0.4676 | 0.029* |
| C16 | 1.04530 (13) | 0.69369 (11) | 0.34475 (9) | 0.0294 (3) |
| H16A | 1.0100 | 0.6930 | 0.2834 | 0.044* |
| H16B | 1.0081 | 0.6141 | 0.3660 | 0.044* |
| H16C | 1.1344 | 0.7160 | 0.3458 | 0.044* |
| C17 | 1.19429 (12) | 0.98323 (12) | 0.42367 (9) | 0.0249 (3) |
| H17A | 1.2378 | 1.0437 | 0.3832 | 0.030* |
| H17B | 1.2438 | 0.9345 | 0.4364 | 0.030* |
| C18 | 1.18373 (13) | 1.04601 (12) | 0.51076 (9) | 0.0338 (4) |
| H18A | 1.1385 | 1.0976 | 0.4980 | 0.051* |
| H18B | 1.2662 | 1.0945 | 0.5398 | 0.051* |
| H18C | 1.1396 | 0.9864 | 0.5507 | 0.051* |
| C19 | 0.65370 (12) | 0.56663 (11) | 0.27664 (9) | 0.0207 (3) |
| C20 | 0.46966 (12) | 0.53325 (11) | 0.17699 (8) | 0.0191 (3) |
| C21 | 0.47506 (12) | 0.38272 (11) | 0.26201 (8) | 0.0206 (3) |
| C22 | 0.59122 (12) | 0.44956 (11) | 0.30103 (9) | 0.0219 (3) |
| H22 | 0.6300 | 0.4173 | 0.3446 | 0.026* |
| C23 | 0.40973 (12) | 0.25534 (11) | 0.28142 (9) | 0.0272 (3) |
| H23A | 0.3253 | 0.2422 | 0.2933 | 0.041* |
| H23B | 0.4532 | 0.2384 | 0.3340 | 0.041* |
| H23C | 0.4080 | 0.2023 | 0.2296 | 0.041* |
| C24 | 0.28663 (12) | 0.50323 (12) | 0.07508 (9) | 0.0267 (3) |
| H24A | 0.2734 | 0.4181 | 0.0787 | 0.032* |
| H24B | 0.2798 | 0.5176 | 0.0109 | 0.032* |
| C25 | 0.18751 (12) | 0.52887 (13) | 0.11996 (10) | 0.0337 (4) |
| H25A | 0.1905 | 0.5100 | 0.1826 | 0.051* |
| H25B | 0.1067 | 0.4798 | 0.0886 | 0.051* |
| H25C | 0.2013 | 0.6135 | 0.1177 | 0.051* |
| C26 | 0.46937 (12) | 0.69518 (11) | 0.08266 (9) | 0.0241 (3) |
| H26A | 0.5203 | 0.7531 | 0.1327 | 0.029* |
| H26B | 0.4049 | 0.7229 | 0.0590 | 0.029* |
| C27 | 0.54991 (13) | 0.69227 (13) | 0.00906 (9) | 0.0344 (4) |
| H27A | 0.6145 | 0.6658 | 0.0324 | 0.052* |
| H27B | 0.5877 | 0.7724 | −0.0112 | 0.052* |
| H27C | 0.4994 | 0.6368 | −0.0414 | 0.052* |
| C28 | 0.60785 (12) | 0.14249 (11) | 0.08855 (9) | 0.0215 (3) |
| C29 | 0.79042 (12) | 0.18576 (11) | 0.01091 (8) | 0.0195 (3) |
| C30 | 0.79382 (12) | 0.31562 (11) | 0.12831 (9) | 0.0211 (3) |
| C31 | 0.67636 (12) | 0.24850 (11) | 0.14345 (9) | 0.0226 (3) |
| H31 | 0.6403 | 0.2730 | 0.1910 | 0.027* |
| C32 | 0.86739 (12) | 0.43106 (11) | 0.18306 (9) | 0.0274 (3) |
| H32A | 0.9365 | 0.4228 | 0.2188 | 0.041* |
| H32B | 0.8148 | 0.4509 | 0.2230 | 0.041* |
| H32C | 0.8989 | 0.4948 | 0.1431 | 0.041* |
| C33 | 0.78135 (12) | 0.04901 (12) | −0.12002 (9) | 0.0267 (3) |
| H33A | 0.7212 | −0.0157 | −0.0905 | 0.032* |

| | | | | |
|---|---|---|---|---|
| H33B | 0.8415 | 0.0185 | −0.1426 | 0.032* |
| C34 | 0.71434 (13) | 0.08240 (12) | −0.19856 (9) | 0.0333 (4) |
| H34A | 0.6490 | 0.1049 | −0.1772 | 0.050* |
| H34B | 0.6782 | 0.0139 | −0.2434 | 0.050* |
| H34C | 0.7727 | 0.1498 | −0.2256 | 0.050* |
| C35 | 0.97244 (12) | 0.22543 (13) | −0.06902 (10) | 0.0315 (4) |
| H35A | 0.9925 | 0.3080 | −0.0432 | 0.038* |
| H35B | 0.9789 | 0.2279 | −0.1343 | 0.038* |
| C36 | 1.06510 (14) | 0.17855 (14) | −0.02713 (10) | 0.0439 (4) |
| H36A | 1.0639 | 0.1822 | 0.0381 | 0.066* |
| H36B | 1.1476 | 0.2276 | −0.0418 | 0.066* |
| H36C | 1.0436 | 0.0957 | −0.0506 | 0.066* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0219 (5) | 0.0236 (5) | 0.0266 (5) | 0.0051 (4) | 0.0046 (4) | −0.0022 (4) |
| O2 | 0.0239 (5) | 0.0237 (5) | 0.0364 (6) | 0.0037 (4) | −0.0077 (4) | 0.0048 (4) |
| O3 | 0.0207 (5) | 0.0229 (5) | 0.0346 (6) | 0.0048 (4) | −0.0045 (4) | 0.0046 (4) |
| O4 | 0.0199 (5) | 0.0280 (5) | 0.0287 (6) | 0.0026 (4) | 0.0066 (4) | −0.0022 (4) |
| N1 | 0.0208 (6) | 0.0154 (6) | 0.0205 (6) | 0.0056 (5) | 0.0012 (5) | −0.0011 (5) |
| N2 | 0.0214 (6) | 0.0188 (6) | 0.0273 (7) | 0.0067 (5) | −0.0026 (5) | −0.0023 (5) |
| N3 | 0.0200 (6) | 0.0210 (6) | 0.0264 (7) | 0.0054 (5) | 0.0043 (5) | 0.0000 (5) |
| N4 | 0.0214 (6) | 0.0155 (6) | 0.0226 (6) | 0.0057 (5) | −0.0006 (5) | 0.0035 (5) |
| N5 | 0.0213 (6) | 0.0173 (6) | 0.0219 (6) | 0.0070 (5) | 0.0011 (5) | 0.0016 (5) |
| N6 | 0.0211 (6) | 0.0190 (6) | 0.0253 (6) | 0.0060 (5) | −0.0019 (5) | 0.0050 (5) |
| N7 | 0.0199 (6) | 0.0209 (6) | 0.0237 (6) | 0.0075 (5) | 0.0029 (5) | 0.0034 (5) |
| N8 | 0.0187 (6) | 0.0189 (6) | 0.0238 (6) | 0.0067 (5) | 0.0016 (5) | 0.0052 (5) |
| N9 | 0.0174 (6) | 0.0224 (6) | 0.0254 (6) | 0.0061 (5) | −0.0008 (5) | 0.0049 (5) |
| N10 | 0.0176 (6) | 0.0183 (6) | 0.0191 (6) | 0.0044 (5) | 0.0017 (5) | −0.0006 (5) |
| N11 | 0.0186 (6) | 0.0209 (6) | 0.0215 (6) | 0.0065 (5) | 0.0008 (5) | 0.0001 (5) |
| N12 | 0.0195 (6) | 0.0243 (6) | 0.0243 (6) | 0.0045 (5) | 0.0055 (5) | −0.0033 (5) |
| C1 | 0.0236 (7) | 0.0197 (7) | 0.0189 (7) | 0.0090 (6) | 0.0002 (6) | 0.0029 (6) |
| C2 | 0.0201 (7) | 0.0213 (7) | 0.0209 (7) | 0.0086 (6) | −0.0016 (6) | 0.0044 (6) |
| C3 | 0.0253 (8) | 0.0180 (7) | 0.0260 (8) | 0.0091 (6) | −0.0048 (6) | −0.0005 (6) |
| C4 | 0.0265 (8) | 0.0207 (7) | 0.0212 (7) | 0.0095 (6) | −0.0004 (6) | −0.0030 (6) |
| C5 | 0.0257 (8) | 0.0239 (8) | 0.0476 (10) | 0.0062 (6) | −0.0046 (7) | −0.0084 (7) |
| C6 | 0.0237 (7) | 0.0227 (7) | 0.0244 (8) | 0.0080 (6) | 0.0028 (6) | −0.0016 (6) |
| C7 | 0.0460 (10) | 0.0270 (8) | 0.0350 (9) | 0.0142 (7) | 0.0019 (7) | 0.0025 (7) |
| C8 | 0.0201 (7) | 0.0304 (8) | 0.0322 (9) | 0.0059 (6) | 0.0044 (6) | −0.0023 (7) |
| C9 | 0.0361 (9) | 0.0243 (8) | 0.0398 (9) | 0.0069 (7) | 0.0137 (7) | 0.0017 (7) |
| C10 | 0.0214 (7) | 0.0226 (7) | 0.0213 (7) | 0.0092 (6) | 0.0000 (6) | 0.0011 (6) |
| C11 | 0.0191 (7) | 0.0211 (7) | 0.0181 (7) | 0.0079 (6) | 0.0024 (5) | 0.0000 (6) |
| C12 | 0.0243 (7) | 0.0209 (7) | 0.0183 (7) | 0.0104 (6) | 0.0031 (6) | 0.0017 (6) |
| C13 | 0.0248 (7) | 0.0201 (7) | 0.0226 (8) | 0.0093 (6) | −0.0009 (6) | 0.0023 (6) |
| C14 | 0.0247 (8) | 0.0200 (7) | 0.0289 (8) | 0.0071 (6) | −0.0007 (6) | 0.0033 (6) |
| C15 | 0.0250 (8) | 0.0217 (7) | 0.0228 (8) | 0.0066 (6) | −0.0034 (6) | 0.0071 (6) |
| C16 | 0.0305 (8) | 0.0223 (8) | 0.0344 (9) | 0.0094 (6) | −0.0014 (7) | 0.0064 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.0202 (7) | 0.0247 (8) | 0.0277 (8) | 0.0070 (6) | −0.0024 (6) | 0.0047 (6) |
| C18 | 0.0319 (9) | 0.0316 (9) | 0.0329 (9) | 0.0089 (7) | −0.0052 (7) | −0.0025 (7) |
| C19 | 0.0194 (7) | 0.0214 (7) | 0.0223 (7) | 0.0091 (6) | 0.0017 (6) | 0.0014 (6) |
| C20 | 0.0184 (7) | 0.0211 (7) | 0.0192 (7) | 0.0089 (6) | 0.0030 (5) | 0.0003 (6) |
| C21 | 0.0215 (7) | 0.0208 (7) | 0.0212 (7) | 0.0097 (6) | 0.0047 (6) | 0.0009 (6) |
| C22 | 0.0218 (7) | 0.0216 (7) | 0.0230 (7) | 0.0092 (6) | 0.0000 (6) | 0.0031 (6) |
| C23 | 0.0231 (8) | 0.0238 (8) | 0.0345 (8) | 0.0082 (6) | 0.0028 (6) | 0.0055 (6) |
| C24 | 0.0206 (7) | 0.0283 (8) | 0.0285 (8) | 0.0074 (6) | −0.0045 (6) | 0.0027 (6) |
| C25 | 0.0204 (8) | 0.0369 (9) | 0.0418 (9) | 0.0086 (7) | 0.0013 (7) | 0.0070 (7) |
| C26 | 0.0217 (7) | 0.0256 (8) | 0.0262 (8) | 0.0102 (6) | 0.0012 (6) | 0.0065 (6) |
| C27 | 0.0326 (9) | 0.0402 (9) | 0.0334 (9) | 0.0156 (7) | 0.0079 (7) | 0.0111 (7) |
| C28 | 0.0204 (7) | 0.0231 (7) | 0.0215 (7) | 0.0086 (6) | 0.0028 (6) | 0.0028 (6) |
| C29 | 0.0176 (7) | 0.0210 (7) | 0.0205 (7) | 0.0075 (6) | 0.0019 (5) | 0.0057 (6) |
| C30 | 0.0216 (7) | 0.0222 (7) | 0.0207 (7) | 0.0104 (6) | −0.0006 (6) | 0.0020 (6) |
| C31 | 0.0213 (7) | 0.0250 (8) | 0.0210 (7) | 0.0084 (6) | 0.0037 (6) | −0.0025 (6) |
| C32 | 0.0233 (8) | 0.0241 (8) | 0.0324 (8) | 0.0072 (6) | 0.0020 (6) | −0.0036 (6) |
| C33 | 0.0241 (8) | 0.0257 (8) | 0.0275 (8) | 0.0065 (6) | 0.0065 (6) | −0.0043 (6) |
| C34 | 0.0325 (9) | 0.0325 (9) | 0.0266 (8) | 0.0026 (7) | 0.0049 (7) | 0.0007 (7) |
| C35 | 0.0217 (8) | 0.0321 (9) | 0.0328 (9) | 0.0007 (6) | 0.0102 (6) | −0.0031 (7) |
| C36 | 0.0233 (8) | 0.0598 (12) | 0.0443 (10) | 0.0130 (8) | 0.0035 (7) | −0.0119 (9) |

*Geometric parameters (Å, °)*

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|---|---|---|---|
| O1—C1 | 1.2506 (15) | C12—C13 | 1.3702 (18) |
| O2—C10 | 1.2459 (15) | C12—C14 | 1.4977 (17) |
| O3—C19 | 1.2451 (15) | C13—H13 | 0.9500 |
| O4—C28 | 1.2477 (15) | C14—H14A | 0.9800 |
| N1—C2 | 1.3699 (16) | C14—H14B | 0.9800 |
| N1—C1 | 1.3886 (17) | C14—H14C | 0.9800 |
| N1—H1A | 0.8800 | C15—C16 | 1.5206 (19) |
| N2—C2 | 1.3284 (16) | C15—H15A | 0.9900 |
| N2—C3 | 1.3628 (17) | C15—H15B | 0.9900 |
| N3—C2 | 1.3445 (17) | C16—H16A | 0.9800 |
| N3—C8 | 1.4677 (16) | C16—H16B | 0.9800 |
| N3—C6 | 1.4692 (16) | C16—H16C | 0.9800 |
| N4—C11 | 1.3732 (16) | C17—C18 | 1.5196 (19) |
| N4—C10 | 1.3956 (16) | C17—H17A | 0.9900 |
| N4—H4A | 0.8800 | C17—H17B | 0.9900 |
| N5—C11 | 1.3311 (16) | C18—H18A | 0.9800 |
| N5—C12 | 1.3658 (16) | C18—H18B | 0.9800 |
| N6—C11 | 1.3504 (16) | C18—H18C | 0.9800 |
| N6—C15 | 1.4676 (16) | C19—C22 | 1.4145 (17) |
| N6—C17 | 1.4691 (16) | C21—C22 | 1.3677 (17) |
| N7—C20 | 1.3301 (16) | C21—C23 | 1.5004 (17) |
| N7—C21 | 1.3645 (16) | C22—H22 | 0.9500 |
| N8—C20 | 1.3698 (16) | C23—H23A | 0.9800 |
| N8—C19 | 1.3963 (16) | C23—H23B | 0.9800 |
| N8—H8C | 0.8800 | C23—H23C | 0.9800 |
| N9—C20 | 1.3517 (16) | C24—C25 | 1.5158 (19) |

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|---|---|---|---|
| N9—C26 | 1.4673 (16) | C24—H24A | 0.9900 |
| N9—C24 | 1.4685 (16) | C24—H24B | 0.9900 |
| N10—C29 | 1.3735 (16) | C25—H25A | 0.9800 |
| N10—C28 | 1.3902 (16) | C25—H25B | 0.9800 |
| N10—H10A | 0.8800 | C25—H25C | 0.9800 |
| N11—C29 | 1.3291 (15) | C26—C27 | 1.5213 (19) |
| N11—C30 | 1.3632 (17) | C26—H26A | 0.9900 |
| N12—C29 | 1.3501 (17) | C26—H26B | 0.9900 |
| N12—C33 | 1.4671 (16) | C27—H27A | 0.9800 |
| N12—C35 | 1.4672 (16) | C27—H27B | 0.9800 |
| C1—C4 | 1.4107 (17) | C27—H27C | 0.9800 |
| C3—C4 | 1.3653 (18) | C28—C31 | 1.4138 (17) |
| C3—C5 | 1.5002 (18) | C30—C31 | 1.3615 (18) |
| C4—H4 | 0.9500 | C30—C32 | 1.5013 (17) |
| C5—H5A | 0.9800 | C31—H31 | 0.9500 |
| C5—H5B | 0.9800 | C32—H32A | 0.9800 |
| C5—H5C | 0.9800 | C32—H32B | 0.9800 |
| C6—C7 | 1.5234 (19) | C32—H32C | 0.9800 |
| C6—H6A | 0.9900 | C33—C34 | 1.5234 (19) |
| C6—H6B | 0.9900 | C33—H33A | 0.9900 |
| C7—H7A | 0.9800 | C33—H33B | 0.9900 |
| C7—H7B | 0.9800 | C34—H34A | 0.9800 |
| C7—H7C | 0.9800 | C34—H34B | 0.9800 |
| C8—C9 | 1.5190 (19) | C34—H34C | 0.9800 |
| C8—H8A | 0.9900 | C35—C36 | 1.519 (2) |
| C8—H8B | 0.9900 | C35—H35A | 0.9900 |
| C9—H9A | 0.9800 | C35—H35B | 0.9900 |
| C9—H9B | 0.9800 | C36—H36A | 0.9800 |
| C9—H9C | 0.9800 | C36—H36B | 0.9800 |
| C10—C13 | 1.4136 (18) | C36—H36C | 0.9800 |
| C2—N1—C1 | 122.70 (11) | H16A—C16—H16C | 109.5 |
| C2—N1—H1A | 118.7 | H16B—C16—H16C | 109.5 |
| C1—N1—H1A | 118.7 | N6—C17—C18 | 111.92 (12) |
| C2—N2—C3 | 116.78 (12) | N6—C17—H17A | 109.2 |
| C2—N3—C8 | 119.26 (11) | C18—C17—H17A | 109.2 |
| C2—N3—C6 | 123.42 (11) | N6—C17—H17B | 109.2 |
| C8—N3—C6 | 117.23 (11) | C18—C17—H17B | 109.2 |
| C11—N4—C10 | 122.46 (11) | H17A—C17—H17B | 107.9 |
| C11—N4—H4A | 118.8 | C17—C18—H18A | 109.5 |
| C10—N4—H4A | 118.8 | C17—C18—H18B | 109.5 |
| C11—N5—C12 | 116.80 (11) | H18A—C18—H18B | 109.5 |
| C11—N6—C15 | 123.21 (11) | C17—C18—H18C | 109.5 |
| C11—N6—C17 | 119.55 (11) | H18A—C18—H18C | 109.5 |
| C15—N6—C17 | 117.07 (10) | H18B—C18—H18C | 109.5 |
| C20—N7—C21 | 116.87 (11) | O3—C19—N8 | 119.03 (12) |
| C20—N8—C19 | 122.58 (11) | O3—C19—C22 | 126.50 (12) |
| C20—N8—H8C | 118.7 | N8—C19—C22 | 114.47 (11) |
| C19—N8—H8C | 118.7 | N7—C20—N9 | 119.12 (12) |
| C20—N9—C26 | 123.02 (11) | N7—C20—N8 | 122.33 (12) |

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| C20—N9—C24 | 120.05 (11) | N9—C20—N8 | 118.55 (12) |
| C26—N9—C24 | 116.67 (11) | N7—C21—C22 | 123.59 (12) |
| C29—N10—C28 | 122.68 (11) | N7—C21—C23 | 114.92 (11) |
| C29—N10—H10A | 118.7 | C22—C21—C23 | 121.45 (12) |
| C28—N10—H10A | 118.7 | C21—C22—C19 | 120.09 (12) |
| C29—N11—C30 | 117.02 (11) | C21—C22—H22 | 120.0 |
| C29—N12—C33 | 123.36 (11) | C19—C22—H22 | 120.0 |
| C29—N12—C35 | 120.25 (11) | C21—C23—H23A | 109.5 |
| C33—N12—C35 | 115.98 (11) | C21—C23—H23B | 109.5 |
| O1—C1—N1 | 118.90 (11) | H23A—C23—H23B | 109.5 |
| O1—C1—C4 | 126.25 (13) | C21—C23—H23C | 109.5 |
| N1—C1—C4 | 114.84 (12) | H23A—C23—H23C | 109.5 |
| N2—C2—N3 | 119.39 (12) | H23B—C23—H23C | 109.5 |
| N2—C2—N1 | 122.02 (13) | N9—C24—C25 | 112.31 (11) |
| N3—C2—N1 | 118.59 (11) | N9—C24—H24A | 109.1 |
| N2—C3—C4 | 123.99 (12) | C25—C24—H24A | 109.1 |
| N2—C3—C5 | 114.65 (13) | N9—C24—H24B | 109.1 |
| C4—C3—C5 | 121.36 (13) | C25—C24—H24B | 109.1 |
| C3—C4—C1 | 119.56 (13) | H24A—C24—H24B | 107.9 |
| C3—C4—H4 | 120.2 | C24—C25—H25A | 109.5 |
| C1—C4—H4 | 120.2 | C24—C25—H25B | 109.5 |
| C3—C5—H5A | 109.5 | H25A—C25—H25B | 109.5 |
| C3—C5—H5B | 109.5 | C24—C25—H25C | 109.5 |
| H5A—C5—H5B | 109.5 | H25A—C25—H25C | 109.5 |
| C3—C5—H5C | 109.5 | H25B—C25—H25C | 109.5 |
| H5A—C5—H5C | 109.5 | N9—C26—C27 | 112.16 (11) |
| H5B—C5—H5C | 109.5 | N9—C26—H26A | 109.2 |
| N3—C6—C7 | 112.06 (11) | C27—C26—H26A | 109.2 |
| N3—C6—H6A | 109.2 | N9—C26—H26B | 109.2 |
| C7—C6—H6A | 109.2 | C27—C26—H26B | 109.2 |
| N3—C6—H6B | 109.2 | H26A—C26—H26B | 107.9 |
| C7—C6—H6B | 109.2 | C26—C27—H27A | 109.5 |
| H6A—C6—H6B | 107.9 | C26—C27—H27B | 109.5 |
| C6—C7—H7A | 109.5 | H27A—C27—H27B | 109.5 |
| C6—C7—H7B | 109.5 | C26—C27—H27C | 109.5 |
| H7A—C7—H7B | 109.5 | H27A—C27—H27C | 109.5 |
| C6—C7—H7C | 109.5 | H27B—C27—H27C | 109.5 |
| H7A—C7—H7C | 109.5 | O4—C28—N10 | 119.22 (12) |
| H7B—C7—H7C | 109.5 | O4—C28—C31 | 126.28 (13) |
| N3—C8—C9 | 111.14 (12) | N10—C28—C31 | 114.48 (12) |
| N3—C8—H8A | 109.4 | N11—C29—N12 | 119.22 (12) |
| C9—C8—H8A | 109.4 | N11—C29—N10 | 121.97 (12) |
| N3—C8—H8B | 109.4 | N12—C29—N10 | 118.80 (11) |
| C9—C8—H8B | 109.4 | C31—C30—N11 | 123.61 (12) |
| H8A—C8—H8B | 108.0 | C31—C30—C32 | 121.54 (12) |
| C8—C9—H9A | 109.5 | N11—C30—C32 | 114.85 (12) |
| C8—C9—H9B | 109.5 | C30—C31—C28 | 120.19 (13) |
| H9A—C9—H9B | 109.5 | C30—C31—H31 | 119.9 |
| C8—C9—H9C | 109.5 | C28—C31—H31 | 119.9 |

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|---|---|---|---|
| H9A—C9—H9C | 109.5 | C30—C32—H32A | 109.5 |
| H9B—C9—H9C | 109.5 | C30—C32—H32B | 109.5 |
| O2—C10—N4 | 118.68 (12) | H32A—C32—H32B | 109.5 |
| O2—C10—C13 | 126.68 (13) | C30—C32—H32C | 109.5 |
| N4—C10—C13 | 114.64 (12) | H32A—C32—H32C | 109.5 |
| N5—C11—N6 | 119.06 (12) | H32B—C32—H32C | 109.5 |
| N5—C11—N4 | 122.39 (12) | N12—C33—C34 | 111.74 (12) |
| N6—C11—N4 | 118.55 (12) | N12—C33—H33A | 109.3 |
| N5—C12—C13 | 123.62 (12) | C34—C33—H33A | 109.3 |
| N5—C12—C14 | 115.00 (11) | N12—C33—H33B | 109.3 |
| C13—C12—C14 | 121.36 (12) | C34—C33—H33B | 109.3 |
| C12—C13—C10 | 120.07 (12) | H33A—C33—H33B | 107.9 |
| C12—C13—H13 | 120.0 | C33—C34—H34A | 109.5 |
| C10—C13—H13 | 120.0 | C33—C34—H34B | 109.5 |
| C12—C14—H14A | 109.5 | H34A—C34—H34B | 109.5 |
| C12—C14—H14B | 109.5 | C33—C34—H34C | 109.5 |
| H14A—C14—H14B | 109.5 | H34A—C34—H34C | 109.5 |
| C12—C14—H14C | 109.5 | H34B—C34—H34C | 109.5 |
| H14A—C14—H14C | 109.5 | N12—C35—C36 | 112.23 (13) |
| H14B—C14—H14C | 109.5 | N12—C35—H35A | 109.2 |
| N6—C15—C16 | 112.98 (12) | C36—C35—H35A | 109.2 |
| N6—C15—H15A | 109.0 | N12—C35—H35B | 109.2 |
| C16—C15—H15A | 109.0 | C36—C35—H35B | 109.2 |
| N6—C15—H15B | 109.0 | H35A—C35—H35B | 107.9 |
| C16—C15—H15B | 109.0 | C35—C36—H36A | 109.5 |
| H15A—C15—H15B | 107.8 | C35—C36—H36B | 109.5 |
| C15—C16—H16A | 109.5 | H36A—C36—H36B | 109.5 |
| C15—C16—H16B | 109.5 | C35—C36—H36C | 109.5 |
| H16A—C16—H16B | 109.5 | H36A—C36—H36C | 109.5 |
| C15—C16—H16C | 109.5 | H36B—C36—H36C | 109.5 |
| C2—N1—C1—O1 | −175.40 (11) | C20—N8—C19—O3 | −178.29 (12) |
| C2—N1—C1—C4 | 3.58 (18) | C20—N8—C19—C22 | 2.09 (18) |
| C3—N2—C2—N3 | 178.60 (12) | C21—N7—C20—N9 | 179.71 (12) |
| C3—N2—C2—N1 | −1.22 (18) | C21—N7—C20—N8 | −0.80 (19) |
| C8—N3—C2—N2 | 6.88 (19) | C26—N9—C20—N7 | −176.98 (12) |
| C6—N3—C2—N2 | −176.70 (11) | C24—N9—C20—N7 | −3.01 (19) |
| C8—N3—C2—N1 | −173.30 (11) | C26—N9—C20—N8 | 3.51 (19) |
| C6—N3—C2—N1 | 3.13 (19) | C24—N9—C20—N8 | 177.48 (11) |
| C1—N1—C2—N2 | −1.2 (2) | C19—N8—C20—N7 | −1.6 (2) |
| C1—N1—C2—N3 | 178.98 (11) | C19—N8—C20—N9 | 177.87 (12) |
| C2—N2—C3—C4 | 1.1 (2) | C20—N7—C21—C22 | 2.7 (2) |
| C2—N2—C3—C5 | −179.06 (12) | C20—N7—C21—C23 | −175.17 (11) |
| N2—C3—C4—C1 | 1.5 (2) | N7—C21—C22—C19 | −2.2 (2) |
| C5—C3—C4—C1 | −178.38 (12) | C23—C21—C22—C19 | 175.57 (12) |
| O1—C1—C4—C3 | 175.25 (13) | O3—C19—C22—C21 | −179.86 (13) |
| N1—C1—C4—C3 | −3.64 (19) | N8—C19—C22—C21 | −0.27 (19) |
| C2—N3—C6—C7 | 81.37 (16) | C20—N9—C24—C25 | 98.62 (15) |
| C8—N3—C6—C7 | −102.13 (15) | C26—N9—C24—C25 | −87.03 (15) |
| C2—N3—C8—C9 | 87.27 (15) | C20—N9—C26—C27 | 80.44 (16) |

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| C6—N3—C8—C9 | −89.38 (14) | C24—N9—C26—C27 | −93.72 (14) |
| C11—N4—C10—O2 | −178.31 (12) | C29—N10—C28—O4 | −179.85 (12) |
| C11—N4—C10—C13 | 1.82 (19) | C29—N10—C28—C31 | 1.71 (18) |
| C12—N5—C11—N6 | −178.93 (12) | C30—N11—C29—N12 | −179.29 (12) |
| C12—N5—C11—N4 | 0.77 (19) | C30—N11—C29—N10 | 0.44 (18) |
| C15—N6—C11—N5 | 175.93 (12) | C33—N12—C29—N11 | −174.42 (12) |
| C17—N6—C11—N5 | 0.78 (19) | C35—N12—C29—N11 | −2.13 (19) |
| C15—N6—C11—N4 | −3.8 (2) | C33—N12—C29—N10 | 5.84 (19) |
| C17—N6—C11—N4 | −178.93 (11) | C35—N12—C29—N10 | 178.13 (12) |
| C10—N4—C11—N5 | −1.9 (2) | C28—N10—C29—N11 | −2.1 (2) |
| C10—N4—C11—N6 | 177.82 (12) | C28—N10—C29—N12 | 177.67 (11) |
| C11—N5—C12—C13 | 0.2 (2) | C29—N11—C30—C31 | 1.41 (19) |
| C11—N5—C12—C14 | 178.47 (11) | C29—N11—C30—C32 | −177.92 (11) |
| N5—C12—C13—C10 | −0.2 (2) | N11—C30—C31—C28 | −1.7 (2) |
| C14—C12—C13—C10 | −178.29 (12) | C32—C30—C31—C28 | 177.60 (12) |
| O2—C10—C13—C12 | 179.31 (14) | O4—C28—C31—C30 | −178.23 (13) |
| N4—C10—C13—C12 | −0.83 (19) | N10—C28—C31—C30 | 0.09 (19) |
| C11—N6—C15—C16 | 89.40 (16) | C29—N12—C33—C34 | 83.51 (15) |
| C17—N6—C15—C16 | −95.34 (14) | C35—N12—C33—C34 | −89.09 (15) |
| C11—N6—C17—C18 | 89.04 (15) | C29—N12—C35—C36 | 100.38 (15) |
| C15—N6—C17—C18 | −86.41 (15) | C33—N12—C35—C36 | −86.78 (15) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1A···O1$^{i}$ | 0.88 | 2.02 | 2.8420 (19) | 156 |
| N4—H4A···O3 | 0.88 | 1.98 | 2.8407 (18) | 164 |
| N8—H8C···O2 | 0.88 | 1.99 | 2.8420 (18) | 162 |
| N10—H10A···O4$^{ii}$ | 0.88 | 1.98 | 2.8248 (18) | 162 |
| C6—H6A···O1$^{i}$ | 0.99 | 2.22 | 3.116 (2) | 150 |
| C15—H15A···O3 | 0.99 | 2.35 | 3.120 (2) | 134 |
| C16—H16B···O1 | 0.98 | 2.58 | 3.507 (2) | 158 |
| C26—H26A···O2 | 0.99 | 2.31 | 3.130 (2) | 139 |
| C33—H33A···O4$^{ii}$ | 0.99 | 2.42 | 3.143 (2) | 130 |

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

**Fig. 1**

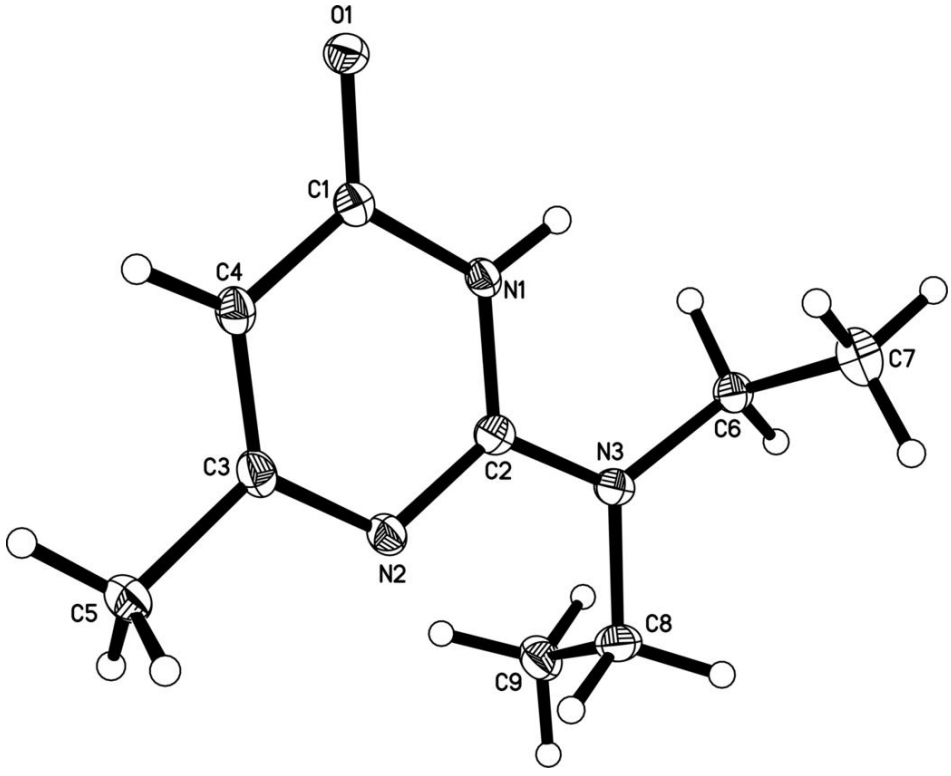

**Fig. 2**