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# 3,5-Dimethoxyacetanilide

**Qing-Lin Lai, Qing-Jie Zhao, Zheng Liu and Jing-Shan Shen***

Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, People's Republic of China
Correspondence e-mail: jsshen@mail.shcnc.ac.cn

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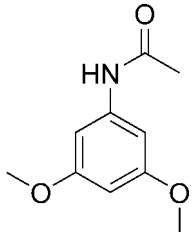
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.108; data-to-parameter ratio = 13.6.

The title compound, $C_{10}H_{13}NO_3$, crystallizes with two molecules in the asymmetric unit. Molecules related by an $a$-axis translation are stacked over each other, bound by $\pi$–$\pi$ interactions with a perpendicular distance of 3.455 Å. Molecules in adjacent stacks are linked to each other through N—H···O hydrogen bonds.

## Related literature

For related literature, see: Allen *et al.* (1987); Hall *et al.* (1992); Hunter & Sanders (1990); Traxler *et al.* (1999).



## Experimental

### *Crystal data*

$C_{10}H_{13}NO_3$
$M_r$ = 195.21
Orthorhombic, *Pbca*
$a$ = 7.1956 (6) Å
$b$ = 16.8320 (14) Å
$c$ = 33.054 (3) Å
$V$ = 4003.4 (6) Å$^3$
$Z$ = 16
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 (2) K
0.30 × 0.20 × 0.20 mm

### *Data collection*

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.972, $T_{max}$ = 0.981
19389 measured reflections
3548 independent reflections
2808 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
$S$ = 1.03
3548 reflections
260 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O6$^{i}$ | 0.86 | 2.03 | 2.8857 (18) | 171 |
| N2—H2$A$···O3$^{ii}$ | 0.86 | 2.17 | 2.9799 (19) | 158 |

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (ii) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

Acknowledgement is made to the crew of Topharman Shanghai Co., Ltd for their active cooperation in this work. We also thank the Instrument Analysis and Research Centre of Shanghai University for the structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2120).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2000). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hall, R. J., Marchant, J., Oliveira-Campos, A. M. F., Queiroz, M.-J. R. P. & Shannon, P. V. R. (1992). *J. Chem. Soc. Perkin Trans. 1*, pp. 3439–3450.
Hunter, C. A. & Sanders, J. K. M. (1990). *J. Am. Chem. Soc.* **112**, 5525–5534.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Traxler, P., Green, J., Mett, H., Séquin, U. & Furet, P. (1999). *J. Med. Chem.* **42**, 1018–1026.

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# supplementary materials

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# 3,5-Dimethoxyacetanilide

**Q.-L. Lai, Q.-J. Zhao, Z. Liu and J.-S. Shen**

## Comment

The title compound, (I), is an important intermediate used to synthesize a variety of pharmaceuticals, such as epidermal growth factor receptor (EGFR) tyrosine kinase inhibitors (Traxler *et al.*, 1999). In our recent research for the synthesis of potential PDE5 inhitiors, 3,5-dimethoxyanilide (I) was synthesized as one of the structural units. We report here the crystal structure of the title compound, which crystallizes with two molecules in the asymmetric unit.

A view of the molecular structure of (I) is depicted in Fig. 1. In the two distinct molecules, the *N*-acetyl group is oriented at angles of 3.10 (2)° and 20.00 (3)° to the aromatic plane. All bond lengths and angles are normal (Allen *et al.*, 1987). Molecules related by an *a*-axis translation are stacked over each other and the perpendicular distance between the stacking planes is 3.455Å (Fig. 2). It is, therefore, inferred that the stacked molecules are bound to each other by π-π interactions (Hunter & Sanders, 1990). The stacked columns are linked together *via* an intermolecular hydrogen bond in which the amide H act as a donor to O atom (Fig. 2 and Table 1).

## Experimental

The title compound was prepared by acetylation of 3,5-dimethoxyaniline according to the method described by Hall *et al.*, (1992). Single crystals suitable for X-ray analysis (m.p. 426 K) were obtained by slow evaporation of a dichloromethane solution at 298 K.

## Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 - 0.96 Å, N—H = 0.86 Å, and $U_{iso} = 1.2U_{eq}$(C) or (N).

## Figures

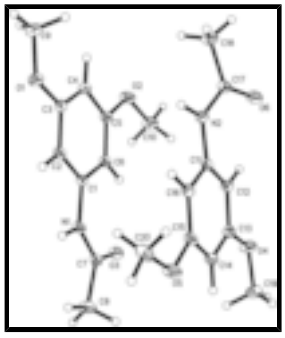

Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

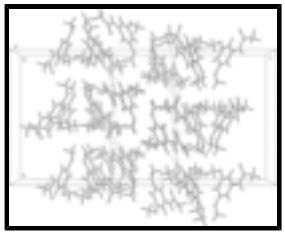

Fig. 2. The crystal packing of (I), viewed along the ⟨i⟩a⟨/i⟩ axis. Hydrogen bonds are shown as dashed lines.

### 3,5-Dimethoxyacetanilide

*Crystal data*

| | |
|---|---|
| $C_{10}H_{13}NO_3$ | $D_x$ = 1.296 Mg m$^{-3}$ |
| $M_r$ = 195.21 | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Orthorhombic, *Pbca* | Cell parameters from 4958 reflections |
| *a* = 7.1956 (6) Å | θ = 2.5–24.7º |
| *b* = 16.8320 (14) Å | μ = 0.10 mm$^{-1}$ |
| *c* = 33.054 (3) Å | *T* = 293 (2) K |
| *V* = 4003.4 (6) Å$^3$ | Block, colourless |
| *Z* = 16 | 0.30 × 0.20 × 0.20 mm |
| $F_{000}$ = 1664 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII diffractometer | 3548 independent reflections |
| Radiation source: fine-focus sealed tube | 2808 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.033 |
| *T* = 298(2) K | $\theta_{max}$ = 25.1º |
| φ and ω scans | $\theta_{min}$ = 2.5º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −8→8 |
| $T_{min}$ = 0.972, $T_{max}$ = 0.981 | *k* = −19→20 |
| 19389 measured reflections | *l* = −30→39 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 1.2714P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.042 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $wR(F^2)$ = 0.108 | $\Delta\rho_{max}$ = 0.25 e Å$^{-3}$ |
| *S* = 1.03 | $\Delta\rho_{min}$ = −0.14 e Å$^{-3}$ |
| 3548 reflections | Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| 260 parameters | Extinction coefficient: 0.0015 (4) |

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

*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 $F^2 > 2\text{sigma}(F^2)$ 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 | 0.9040 (2) | 0.66216 (10) | 0.91166 (5) | 0.0360 (4) |
| C2 | 0.7495 (2) | 0.70799 (10) | 0.92004 (5) | 0.0416 (4) |
| H2 | 0.7399 | 0.7590 | 0.9095 | 0.050* |
| C3 | 0.6087 (2) | 0.67783 (11) | 0.94428 (5) | 0.0430 (4) |
| C4 | 0.6212 (3) | 0.60184 (11) | 0.96012 (5) | 0.0464 (5) |
| H4 | 0.5277 | 0.5817 | 0.9766 | 0.056* |
| C5 | 0.7761 (3) | 0.55664 (10) | 0.95083 (5) | 0.0428 (4) |
| C6 | 0.9191 (2) | 0.58522 (10) | 0.92700 (5) | 0.0404 (4) |
| H6 | 1.0226 | 0.5540 | 0.9214 | 0.048* |
| C7 | 1.2042 (2) | 0.66862 (10) | 0.87336 (5) | 0.0410 (4) |
| C8 | 1.3073 (3) | 0.72307 (12) | 0.84542 (7) | 0.0596 (6) |
| H8A | 1.4291 | 0.7331 | 0.8561 | 0.089* |
| H8B | 1.2409 | 0.7723 | 0.8430 | 0.089* |
| H8C | 1.3181 | 0.6987 | 0.8193 | 0.089* |
| C9 | 0.3195 (3) | 0.70352 (14) | 0.97704 (7) | 0.0659 (6) |
| H9A | 0.2630 | 0.6562 | 0.9665 | 0.099* |
| H9B | 0.2275 | 0.7446 | 0.9792 | 0.099* |
| H9C | 0.3705 | 0.6926 | 1.0033 | 0.099* |
| C10 | 0.9237 (3) | 0.42958 (11) | 0.95603 (7) | 0.0647 (6) |
| H10A | 0.9281 | 0.4240 | 0.9271 | 0.097* |
| H10B | 0.9047 | 0.3784 | 0.9682 | 0.097* |
| H10C | 1.0388 | 0.4516 | 0.9655 | 0.097* |
| C11 | 0.7292 (2) | 0.50583 (10) | 0.83936 (5) | 0.0371 (4) |
| C12 | 0.8709 (2) | 0.45172 (10) | 0.83355 (5) | 0.0412 (4) |
| H12 | 0.8650 | 0.4016 | 0.8454 | 0.049* |
| C13 | 1.0227 (2) | 0.47288 (10) | 0.80982 (5) | 0.0420 (4) |
| C14 | 1.0337 (3) | 0.54668 (11) | 0.79191 (5) | 0.0460 (4) |
| H14 | 1.1359 | 0.5604 | 0.7761 | 0.055* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.8897 (3) | 0.60002 (10) | 0.79786 (5) | 0.0454 (5) |
| C16 | 0.7373 (3) | 0.58076 (10) | 0.82121 (5) | 0.0426 (4) |
| H16 | 0.6414 | 0.6171 | 0.8248 | 0.051* |
| C17 | 0.5121 (2) | 0.41904 (10) | 0.87722 (5) | 0.0424 (4) |
| C18 | 0.3505 (3) | 0.42184 (12) | 0.90562 (7) | 0.0607 (6) |
| H18A | 0.2966 | 0.3698 | 0.9078 | 0.091* |
| H18B | 0.2591 | 0.4583 | 0.8955 | 0.091* |
| H18C | 0.3919 | 0.4392 | 0.9318 | 0.091* |
| C19 | 1.3080 (3) | 0.43027 (14) | 0.78001 (6) | 0.0651 (6) |
| H19A | 1.2630 | 0.4393 | 0.7530 | 0.098* |
| H19B | 1.3903 | 0.3854 | 0.7800 | 0.098* |
| H19C | 1.3736 | 0.4765 | 0.7893 | 0.098* |
| C20 | 0.7776 (3) | 0.73162 (12) | 0.78511 (7) | 0.0663 (6) |
| H20A | 0.6589 | 0.7135 | 0.7756 | 0.099* |
| H20B | 0.8127 | 0.7787 | 0.7706 | 0.099* |
| H20C | 0.7697 | 0.7434 | 0.8135 | 0.099* |
| N1 | 1.03993 (19) | 0.69747 (8) | 0.88680 (4) | 0.0405 (4) |
| H1 | 1.0144 | 0.7449 | 0.8789 | 0.049* |
| N2 | 0.5737 (2) | 0.49023 (8) | 0.86409 (4) | 0.0418 (4) |
| H2A | 0.5105 | 0.5310 | 0.8717 | 0.050* |
| O1 | 0.46382 (18) | 0.72883 (8) | 0.95061 (4) | 0.0596 (4) |
| O2 | 0.77427 (19) | 0.48116 (8) | 0.96687 (4) | 0.0603 (4) |
| O3 | 1.26690 (17) | 0.60353 (7) | 0.88250 (4) | 0.0516 (4) |
| O4 | 1.15542 (19) | 0.41493 (8) | 0.80618 (4) | 0.0606 (4) |
| O5 | 0.9123 (2) | 0.67166 (8) | 0.77872 (5) | 0.0684 (4) |
| O6 | 0.58211 (19) | 0.35588 (7) | 0.86658 (4) | 0.0593 (4) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0339 (9) | 0.0350 (9) | 0.0390 (9) | −0.0056 (7) | −0.0013 (7) | 0.0005 (7) |
| C2 | 0.0427 (10) | 0.0338 (9) | 0.0483 (10) | −0.0018 (8) | 0.0016 (8) | 0.0004 (8) |
| C3 | 0.0389 (10) | 0.0420 (10) | 0.0481 (10) | −0.0026 (8) | 0.0049 (8) | −0.0096 (8) |
| C4 | 0.0449 (11) | 0.0473 (11) | 0.0472 (11) | −0.0106 (9) | 0.0100 (9) | −0.0012 (9) |
| C5 | 0.0464 (10) | 0.0379 (10) | 0.0442 (10) | −0.0077 (8) | 0.0019 (9) | 0.0046 (8) |
| C6 | 0.0393 (9) | 0.0346 (9) | 0.0472 (10) | −0.0029 (8) | 0.0015 (8) | 0.0032 (8) |
| C7 | 0.0388 (9) | 0.0355 (10) | 0.0488 (10) | −0.0020 (8) | 0.0023 (8) | 0.0045 (8) |
| C8 | 0.0496 (12) | 0.0519 (12) | 0.0772 (14) | 0.0034 (10) | 0.0167 (11) | 0.0182 (10) |
| C9 | 0.0507 (12) | 0.0783 (16) | 0.0687 (14) | −0.0001 (11) | 0.0212 (11) | −0.0086 (12) |
| C10 | 0.0717 (14) | 0.0412 (11) | 0.0811 (15) | 0.0054 (10) | 0.0221 (12) | 0.0182 (10) |
| C11 | 0.0434 (10) | 0.0345 (9) | 0.0334 (9) | −0.0049 (8) | 0.0004 (8) | −0.0004 (7) |
| C12 | 0.0476 (10) | 0.0356 (9) | 0.0402 (10) | −0.0011 (8) | 0.0036 (8) | 0.0060 (8) |
| C13 | 0.0433 (10) | 0.0430 (10) | 0.0395 (10) | 0.0013 (8) | 0.0008 (8) | 0.0013 (8) |
| C14 | 0.0432 (10) | 0.0491 (11) | 0.0458 (10) | −0.0093 (9) | 0.0047 (8) | 0.0052 (9) |
| C15 | 0.0540 (11) | 0.0349 (10) | 0.0473 (10) | −0.0089 (9) | −0.0012 (9) | 0.0072 (8) |
| C16 | 0.0475 (10) | 0.0328 (9) | 0.0474 (10) | −0.0007 (8) | 0.0019 (9) | 0.0020 (8) |
| C17 | 0.0418 (10) | 0.0371 (10) | 0.0484 (11) | −0.0006 (8) | 0.0018 (9) | 0.0091 (8) |
| C18 | 0.0609 (13) | 0.0515 (12) | 0.0698 (14) | 0.0009 (10) | 0.0218 (11) | 0.0146 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C19 | 0.0476 (12) | 0.0824 (16) | 0.0652 (14) | 0.0079 (11) | 0.0153 (11) | 0.0046 (12) |
| C20 | 0.0742 (15) | 0.0407 (11) | 0.0838 (16) | −0.0050 (11) | −0.0032 (13) | 0.0169 (11) |
| N1 | 0.0377 (8) | 0.0306 (7) | 0.0533 (9) | 0.0007 (6) | 0.0051 (7) | 0.0097 (6) |
| N2 | 0.0471 (9) | 0.0312 (8) | 0.0473 (9) | 0.0012 (7) | 0.0114 (7) | 0.0023 (6) |
| O1 | 0.0494 (8) | 0.0505 (8) | 0.0788 (10) | 0.0038 (6) | 0.0238 (7) | −0.0031 (7) |
| O2 | 0.0619 (9) | 0.0446 (8) | 0.0742 (9) | −0.0014 (7) | 0.0207 (8) | 0.0197 (7) |
| O3 | 0.0492 (8) | 0.0363 (7) | 0.0694 (9) | 0.0076 (6) | 0.0107 (7) | 0.0104 (6) |
| O4 | 0.0530 (8) | 0.0597 (9) | 0.0691 (9) | 0.0127 (7) | 0.0207 (7) | 0.0153 (7) |
| O5 | 0.0704 (10) | 0.0442 (8) | 0.0907 (11) | −0.0032 (7) | 0.0199 (8) | 0.0249 (7) |
| O6 | 0.0538 (8) | 0.0321 (7) | 0.0920 (11) | 0.0036 (6) | 0.0194 (8) | 0.0095 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.381 (2) | C11—C16 | 1.398 (2) |
| C1—C6 | 1.395 (2) | C11—N2 | 1.410 (2) |
| C1—N1 | 1.409 (2) | C12—C13 | 1.391 (2) |
| C2—C3 | 1.388 (2) | C12—H12 | 0.9300 |
| C2—H2 | 0.9300 | C13—O4 | 1.371 (2) |
| C3—O1 | 1.366 (2) | C13—C14 | 1.378 (2) |
| C3—C4 | 1.385 (3) | C14—C15 | 1.385 (3) |
| C4—C5 | 1.384 (3) | C14—H14 | 0.9300 |
| C4—H4 | 0.9300 | C15—O5 | 1.371 (2) |
| C5—O2 | 1.377 (2) | C15—C16 | 1.379 (2) |
| C5—C6 | 1.382 (2) | C16—H16 | 0.9300 |
| C6—H6 | 0.9300 | C17—O6 | 1.228 (2) |
| C7—O3 | 1.223 (2) | C17—N2 | 1.349 (2) |
| C7—N1 | 1.353 (2) | C17—C18 | 1.495 (3) |
| C7—C8 | 1.498 (2) | C18—H18A | 0.9600 |
| C8—H8A | 0.9600 | C18—H18B | 0.9600 |
| C8—H8B | 0.9600 | C18—H18C | 0.9600 |
| C8—H8C | 0.9600 | C19—O4 | 1.421 (2) |
| C9—O1 | 1.423 (2) | C19—H19A | 0.9600 |
| C9—H9A | 0.9600 | C19—H19B | 0.9600 |
| C9—H9B | 0.9600 | C19—H19C | 0.9600 |
| C9—H9C | 0.9600 | C20—O5 | 1.415 (3) |
| C10—O2 | 1.428 (2) | C20—H20A | 0.9600 |
| C10—H10A | 0.9600 | C20—H20B | 0.9600 |
| C10—H10B | 0.9600 | C20—H20C | 0.9600 |
| C10—H10C | 0.9600 | N1—H1 | 0.8600 |
| C11—C12 | 1.381 (2) | N2—H2A | 0.8600 |
| C2—C1—C6 | 120.54 (16) | C13—C12—H12 | 120.3 |
| C2—C1—N1 | 116.11 (14) | O4—C13—C14 | 124.29 (16) |
| C6—C1—N1 | 123.34 (15) | O4—C13—C12 | 114.49 (15) |
| C1—C2—C3 | 119.96 (16) | C14—C13—C12 | 121.23 (17) |
| C1—C2—H2 | 120.0 | C13—C14—C15 | 118.67 (17) |
| C3—C2—H2 | 120.0 | C13—C14—H14 | 120.7 |
| O1—C3—C4 | 124.89 (16) | C15—C14—H14 | 120.7 |
| O1—C3—C2 | 114.56 (16) | O5—C15—C16 | 124.01 (17) |
| C4—C3—C2 | 120.56 (17) | O5—C15—C14 | 114.53 (16) |

| | | | |
|---|---|---|---|
| C5—C4—C3 | 118.43 (16) | C16—C15—C14 | 121.46 (16) |
| C5—C4—H4 | 120.8 | C15—C16—C11 | 119.05 (17) |
| C3—C4—H4 | 120.8 | C15—C16—H16 | 120.5 |
| O2—C5—C6 | 123.21 (16) | C11—C16—H16 | 120.5 |
| O2—C5—C4 | 114.46 (16) | O6—C17—N2 | 122.81 (16) |
| C6—C5—C4 | 122.32 (16) | O6—C17—C18 | 121.76 (16) |
| C5—C6—C1 | 118.18 (16) | N2—C17—C18 | 115.43 (16) |
| C5—C6—H6 | 120.9 | C17—C18—H18A | 109.5 |
| C1—C6—H6 | 120.9 | C17—C18—H18B | 109.5 |
| O3—C7—N1 | 124.26 (16) | H18A—C18—H18B | 109.5 |
| O3—C7—C8 | 121.16 (16) | C17—C18—H18C | 109.5 |
| N1—C7—C8 | 114.57 (15) | H18A—C18—H18C | 109.5 |
| C7—C8—H8A | 109.5 | H18B—C18—H18C | 109.5 |
| C7—C8—H8B | 109.5 | O4—C19—H19A | 109.5 |
| H8A—C8—H8B | 109.5 | O4—C19—H19B | 109.5 |
| C7—C8—H8C | 109.5 | H19A—C19—H19B | 109.5 |
| H8A—C8—H8C | 109.5 | O4—C19—H19C | 109.5 |
| H8B—C8—H8C | 109.5 | H19A—C19—H19C | 109.5 |
| O1—C9—H9A | 109.5 | H19B—C19—H19C | 109.5 |
| O1—C9—H9B | 109.5 | O5—C20—H20A | 109.5 |
| H9A—C9—H9B | 109.5 | O5—C20—H20B | 109.5 |
| O1—C9—H9C | 109.5 | H20A—C20—H20B | 109.5 |
| H9A—C9—H9C | 109.5 | O5—C20—H20C | 109.5 |
| H9B—C9—H9C | 109.5 | H20A—C20—H20C | 109.5 |
| O2—C10—H10A | 109.5 | H20B—C20—H20C | 109.5 |
| O2—C10—H10B | 109.5 | C7—N1—C1 | 130.28 (14) |
| H10A—C10—H10B | 109.5 | C7—N1—H1 | 114.9 |
| O2—C10—H10C | 109.5 | C1—N1—H1 | 114.9 |
| H10A—C10—H10C | 109.5 | C17—N2—C11 | 127.76 (15) |
| H10B—C10—H10C | 109.5 | C17—N2—H2A | 116.1 |
| C12—C11—C16 | 120.29 (16) | C11—N2—H2A | 116.1 |
| C12—C11—N2 | 122.95 (15) | C3—O1—C9 | 117.57 (16) |
| C16—C11—N2 | 116.74 (15) | C5—O2—C10 | 117.22 (14) |
| C11—C12—C13 | 119.30 (16) | C13—O4—C19 | 117.55 (15) |
| C11—C12—H12 | 120.3 | C15—O5—C20 | 118.46 (16) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O6$^{i}$ | 0.86 | 2.03 | 2.8857 (18) | 171 |
| N2—H2A···O3$^{ii}$ | 0.86 | 2.17 | 2.9799 (19) | 158 |

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*; (ii) *x*−1, *y*, *z*.

**Fig. 1**

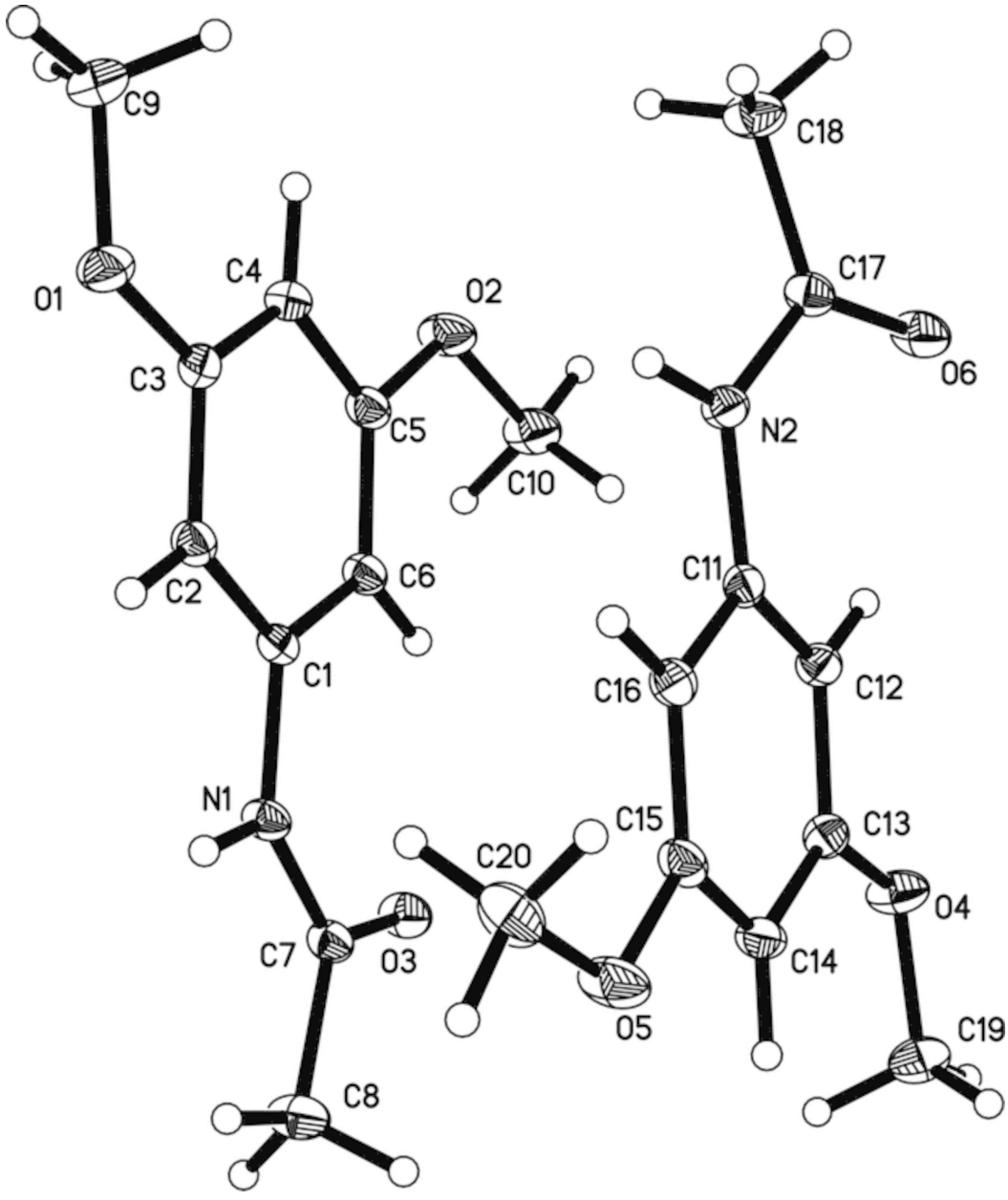
C9
O1
C4
O2
C3
C5
C10
C2
C6
C1
N1
C7
O3
C8
C18
C17
O6
N2
C11
C16
C12
C15
C13
C20
O4
C14
O5
C19

**Fig. 2**