

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1,3-Bis(4-methoxybenzyl)-6-methylpyrimidine-2,4(1*H*,3*H*)-dione

Gong-Chun Li, Li-Ke Zhang, Zhi-Yu Ju and Feng-Ling Yang*

College of Chemistry and Chemical Engineering, Xuchang University, Xuchang, Henan Province 461000, People's Republic of China
Correspondence e-mail: actaeli@gmail.com

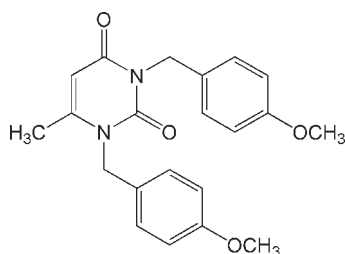
Received 10 June 2010; accepted 24 June 2010

Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.096; data-to-parameter ratio = 17.2.

The title compound, $\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}_4$, was prepared by reaction of 6-methylpyrimidine-2,4(1*H*,3*H*)-dione and 1-chloromethyl-4-methoxybenzene. In the title molecule, the central pyrimidine ring forms dihedral angles of 62.16 (4) and 69.77 (3)° with the two benzene rings. In the crystal, weak intermolecular C—H···O hydrogen bonds link the molecules into chains.

Related literature

For the applications of pyrimidine derivatives as pesticides and pharmaceutical agents, see: Condon *et al.* (1993); as agrochemicals, see: Maeno *et al.* (1990); as antiviral agents, see: Gilchrist (1997); as herbicides, see: Selby *et al.* (2002); Zhu *et al.* (2007). For a related structure, see: Yang & Li (2006).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}_4$	$V = 1787.5$ (3) Å ³
$M_r = 366.41$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.4133$ (9) Å	$\mu = 0.10$ mm ⁻¹
$b = 9.929$ (1) Å	$T = 113$ K
$c = 21.407$ (3) Å	$0.26 \times 0.24 \times 0.22$ mm
$\beta = 91.614$ (4)°	

Data collection

Rigaku Saturn724 CCD diffractometer	17394 measured reflections
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MS, 2009)	4250 independent reflections
$T_{\min} = 0.976$, $T_{\max} = 0.979$	3035 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	247 parameters
$wR(F^2) = 0.096$	H-atom parameters constrained
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.29$ e Å ⁻³
4250 reflections	$\Delta\rho_{\text{min}} = -0.16$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C20}-\text{H20}\cdots\text{O3}^i$	0.95	2.51	3.3627 (14)	150

Symmetry code: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MS, 2009); 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: *CrystalStructure* (Rigaku/MS, 2009); software used to prepare material for publication: *CrystalStructure*.

This work was supported by the Program for New Century Excellent Talents at the University of Henan Province (No. 2005HANCET-17), the Natural Science Foundation of Henan Province, China (grant No. 082300420110) and the Natural Science Foundation of Henan Province Education Department, China (grant No. 2007150036).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2250).

References

- Condon, M. E., Brady, T. E., Feist, D., Malefy, T., Marc, P., Quakenbush, L. S., Rodaway, S. J., Shaner, D. L. & Teale, B. (1993). *Brighton Crop Protection Conference on Weeds*, pp. 41–46. Alton, Hampshire, England: BCPC Publications.
- Gilchrist, T. L. (1997). *Heterocyclic Chemistry*, 3rd ed., pp. 261–276. Singapore: Addison Wesley Longman.
- Maeno, S., Miura, I., Masuda, K. & Nagata, T. (1990). *Brighton Crop Protection Conference on Pests and Diseases*, pp. 415–422. Alton, Hampshire, England: BCPC Publications.
- Rigaku/MS (2009). *CrystalClear* and *CrystalStructure*. Rigaku/MS, The Woodlands, Texas, USA.
- Selby, T. P., Drumm, J. E., Coats, R. A., Coppo, F. T., Gee, S. K., Hay, J. V., Pasteris, R. J. & Stevenson, T. M. (2002). *ACS Symposium Series*, Vol. 800, *Synthesis and Chemistry of Agrochemicals VI*, pp. 74–84. Washington DC: American Chemical Society.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Yang, F.-L. & Li, G.-C. (2006). *Acta Cryst.* **E62**, o3405–o3406.
- Zhu, Y.-Q., Zou, X.-M., Li, G.-C., Yao, C.-S. & Yang, H.-Z. (2007). *Chin. J. Org. Chem.* **27**, 753–757.

supplementary materials

Acta Cryst. (2010). E66, o1858 [doi:10.1107/S1600536810024815]

1,3-Bis(4-methoxybenzyl)-6-methylpyrimidine-2,4(1*H*,3*H*)-dione

G.-C. Li, L.-K. Zhang, Z.-Y. Ju and F.-L. Yang

Comment

Pyrimidine derivatives are very important molecules in biology and have many applications in the areas of pesticide and pharmaceutical agents (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT, which is the most widely used anti-AIDS drug (Gilchrist, 1997). Recently, a new series of highly active herbicides of substituted pyrimidines were reported (Selby *et al.*, 2002); (Zhu *et al.*, 2007), and we have previously reported a related structure (Yang & Li 2006). As part of our goal to discover further biologically active pyrimidine compounds, the title compound was synthesized and its crystal structure determined (Fig. 1).

In the title molecule, the central pyrimidine ring forms dihedral angles of 62.16 (4) and 69.77 (3)° with the two benzene rings. In the crystal, weak intermolecular C—H···O hydrogen bonds link molecules.

Experimental

6-methylpyrimidine-2,4(1*H*,3*H*)-dione (0.63 g, 5 mmol) and anhydrous potassium carbonate (0.84 g, 6 mmol) were mixed in dimethylformamide (20 ml). A solution of 1-(chloromethyl)-4-methoxybenzene (0.79 g, 5 mmol) in acetone (10 ml) was then added dropwise, with stirring at room temperature, and the mixture was stirred for another 10 h and then refluxed for 4 h. The solvent was evaporated *in vacuo* and the residue was washed with water. The resulting white precipitate was recrystallized from ethanol and single crystals were obtained by slow evaporation.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.95 Å, 0.98 Å or 0.99 Å, and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

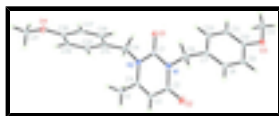


Fig. 1. The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 30% probability level.

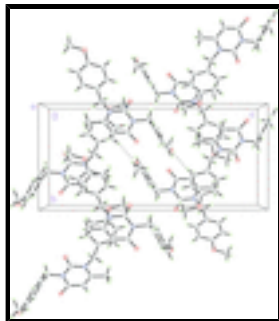


Fig. 2. A packing diagram of the title compound viewed down the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

1,3-Bis(4-methoxybenzyl)-6-methylpyrimidine-2,4(1*H*,3*H*)-dione

Crystal data

$C_{21}H_{22}N_2O_4$	$F(000) = 776$
$M_r = 366.41$	$D_x = 1.361 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$
Hall symbol: $-P\ 2_1/n$	Cell parameters from 5810 reflections
$a = 8.4133 (9) \text{ \AA}$	$\theta = 1.9\text{--}28.0^\circ$
$b = 9.929 (1) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 21.407 (3) \text{ \AA}$	$T = 113 \text{ K}$
$\beta = 91.614 (4)^\circ$	Prism, colorless
$V = 1787.5 (3) \text{ \AA}^3$	$0.26 \times 0.24 \times 0.22 \text{ mm}$
$Z = 4$	

Data collection

Rigaku Saturn724 CCD diffractometer	4250 independent reflections
Radiation source: fine-focus sealed tube graphite	3035 reflections with $I > 2\sigma(I)$
Detector resolution: $14.222 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.037$
ω scans	$\theta_{\text{max}} = 27.9^\circ$, $\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MS, 2009)	$h = -9 \rightarrow 11$
$T_{\text{min}} = 0.976$, $T_{\text{max}} = 0.979$	$k = -12 \rightarrow 13$
17394 measured reflections	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.096$	H-atom parameters constrained
$S = 0.98$	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2]$

4250 reflections
247 parameters
0 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.16 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.77270 (10)	-0.03179 (8)	0.39409 (4)	0.0326 (2)
O2	1.05849 (10)	0.35414 (9)	0.42566 (4)	0.0349 (2)
O3	0.38155 (9)	0.43800 (8)	0.57937 (3)	0.0258 (2)
O4	1.17640 (10)	-0.48075 (8)	0.20574 (4)	0.0286 (2)
N1	0.91553 (10)	0.16121 (9)	0.41019 (4)	0.0235 (2)
N2	0.87518 (10)	0.07201 (9)	0.30901 (4)	0.0231 (2)
C1	0.84910 (13)	0.06125 (12)	0.37267 (5)	0.0244 (3)
C2	1.00559 (13)	0.27014 (12)	0.38848 (5)	0.0257 (3)
C3	1.02826 (13)	0.27076 (12)	0.32258 (5)	0.0257 (3)
H3	1.0893	0.3408	0.3049	0.031*
C4	0.96571 (13)	0.17502 (11)	0.28489 (5)	0.0234 (2)
C5	0.99072 (15)	0.17657 (13)	0.21620 (5)	0.0304 (3)
H5A	1.0646	0.2492	0.2061	0.037*
H5B	0.8888	0.1915	0.1940	0.037*
H5C	1.0353	0.0900	0.2034	0.037*
C6	0.89544 (14)	0.14901 (13)	0.47867 (5)	0.0275 (3)
H6A	0.9940	0.1808	0.5003	0.033*
H6B	0.8820	0.0526	0.4891	0.033*
C7	0.75633 (13)	0.22666 (12)	0.50352 (5)	0.0229 (3)
C8	0.77921 (13)	0.34760 (12)	0.53566 (5)	0.0244 (3)
H8	0.8833	0.3838	0.5406	0.029*
C9	0.65212 (13)	0.41528 (12)	0.56044 (5)	0.0240 (3)
H9	0.6692	0.4972	0.5825	0.029*
C10	0.49895 (13)	0.36351 (11)	0.55308 (5)	0.0213 (2)
C11	0.47377 (14)	0.24358 (12)	0.52095 (5)	0.0250 (3)
H11	0.3694	0.2080	0.5156	0.030*
C12	0.60341 (13)	0.17605 (12)	0.49672 (5)	0.0248 (3)
H12	0.5866	0.0935	0.4751	0.030*

supplementary materials

C13	0.22263 (13)	0.38888 (13)	0.57144 (6)	0.0292 (3)
H13A	0.1932	0.3867	0.5268	0.035*
H13B	0.1497	0.4485	0.5933	0.035*
H13C	0.2160	0.2978	0.5888	0.035*
C14	0.79638 (13)	-0.02957 (12)	0.26809 (6)	0.0263 (3)
H14A	0.7576	0.0153	0.2293	0.032*
H14B	0.7027	-0.0656	0.2895	0.032*
C15	0.90264 (13)	-0.14602 (11)	0.25073 (5)	0.0224 (2)
C16	0.97928 (13)	-0.22551 (12)	0.29611 (5)	0.0236 (3)
H16	0.9686	-0.2036	0.3390	0.028*
C17	1.06997 (13)	-0.33503 (12)	0.28015 (5)	0.0243 (3)
H17	1.1212	-0.3876	0.3118	0.029*
C18	1.08652 (13)	-0.36866 (11)	0.21741 (5)	0.0224 (2)
C19	1.01334 (13)	-0.28976 (12)	0.17146 (5)	0.0251 (3)
H19	1.0255	-0.3107	0.1286	0.030*
C20	0.92206 (13)	-0.17982 (12)	0.18864 (5)	0.0249 (3)
H20	0.8717	-0.1265	0.1570	0.030*
C21	1.18686 (15)	-0.52057 (13)	0.14183 (5)	0.0324 (3)
H21A	1.0798	-0.5359	0.1241	0.039*
H21B	1.2489	-0.6038	0.1393	0.039*
H21C	1.2391	-0.4493	0.1183	0.039*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0372 (5)	0.0225 (5)	0.0387 (5)	-0.0028 (4)	0.0125 (4)	-0.0013 (4)
O2	0.0361 (5)	0.0325 (5)	0.0360 (5)	-0.0066 (4)	-0.0008 (4)	-0.0107 (4)
O3	0.0232 (4)	0.0286 (5)	0.0256 (4)	0.0020 (3)	0.0020 (3)	-0.0037 (3)
O4	0.0340 (5)	0.0237 (5)	0.0280 (4)	0.0067 (4)	0.0025 (3)	-0.0041 (3)
N1	0.0242 (5)	0.0204 (5)	0.0259 (5)	0.0032 (4)	0.0031 (4)	-0.0023 (4)
N2	0.0226 (5)	0.0181 (5)	0.0287 (5)	0.0000 (4)	0.0040 (4)	-0.0044 (4)
C1	0.0224 (6)	0.0187 (6)	0.0322 (6)	0.0036 (5)	0.0054 (5)	-0.0008 (5)
C2	0.0213 (6)	0.0224 (6)	0.0334 (6)	0.0026 (5)	0.0004 (5)	-0.0041 (5)
C3	0.0240 (6)	0.0204 (6)	0.0328 (6)	-0.0003 (5)	0.0053 (5)	-0.0014 (5)
C4	0.0197 (6)	0.0202 (6)	0.0305 (6)	0.0034 (5)	0.0037 (4)	0.0000 (5)
C5	0.0354 (7)	0.0269 (7)	0.0292 (6)	-0.0024 (5)	0.0058 (5)	-0.0024 (5)
C6	0.0286 (6)	0.0266 (7)	0.0274 (6)	0.0056 (5)	0.0003 (5)	0.0015 (5)
C7	0.0267 (6)	0.0223 (6)	0.0197 (5)	0.0022 (5)	0.0012 (4)	0.0043 (4)
C8	0.0225 (6)	0.0276 (7)	0.0229 (6)	-0.0012 (5)	-0.0011 (4)	0.0016 (5)
C9	0.0285 (6)	0.0222 (6)	0.0212 (6)	-0.0012 (5)	-0.0009 (4)	-0.0016 (4)
C10	0.0252 (6)	0.0232 (6)	0.0158 (5)	0.0029 (5)	0.0022 (4)	0.0025 (4)
C11	0.0238 (6)	0.0279 (7)	0.0233 (6)	-0.0039 (5)	0.0012 (4)	0.0000 (5)
C12	0.0317 (6)	0.0214 (6)	0.0214 (5)	-0.0007 (5)	0.0024 (5)	-0.0005 (5)
C13	0.0234 (6)	0.0330 (7)	0.0316 (6)	0.0002 (5)	0.0049 (5)	0.0002 (5)
C14	0.0236 (6)	0.0220 (6)	0.0334 (6)	-0.0016 (5)	0.0003 (5)	-0.0049 (5)
C15	0.0196 (6)	0.0174 (6)	0.0303 (6)	-0.0033 (4)	0.0022 (4)	-0.0034 (5)
C16	0.0257 (6)	0.0228 (6)	0.0225 (5)	-0.0043 (5)	0.0036 (4)	-0.0023 (5)
C17	0.0264 (6)	0.0226 (6)	0.0237 (6)	-0.0017 (5)	-0.0008 (4)	0.0015 (5)

C18	0.0223 (6)	0.0173 (6)	0.0277 (6)	-0.0022 (5)	0.0027 (4)	-0.0023 (5)
C19	0.0301 (6)	0.0234 (6)	0.0217 (6)	-0.0025 (5)	0.0010 (4)	-0.0031 (5)
C20	0.0278 (6)	0.0209 (6)	0.0260 (6)	-0.0004 (5)	-0.0029 (4)	0.0016 (5)
C21	0.0394 (7)	0.0273 (7)	0.0309 (7)	0.0042 (6)	0.0067 (5)	-0.0069 (5)

Geometric parameters (Å, °)

O1—C1	1.2220 (13)	C9—C10	1.3922 (15)
O2—C2	1.2276 (14)	C9—H9	0.9500
O3—C10	1.3677 (13)	C10—C11	1.3886 (16)
O3—C13	1.4288 (13)	C11—C12	1.3929 (15)
O4—C18	1.3723 (13)	C11—H11	0.9500
O4—C21	1.4292 (14)	C12—H12	0.9500
N1—C1	1.3848 (15)	C13—H13A	0.9800
N1—C2	1.4070 (15)	C13—H13B	0.9800
N1—C6	1.4853 (14)	C13—H13C	0.9800
N2—C4	1.3838 (14)	C14—C15	1.5142 (15)
N2—C1	1.3904 (14)	C14—H14A	0.9900
N2—C14	1.4803 (14)	C14—H14B	0.9900
C2—C3	1.4290 (15)	C15—C20	1.3850 (15)
C3—C4	1.3444 (16)	C15—C16	1.3954 (16)
C3—H3	0.9500	C16—C17	1.3770 (16)
C4—C5	1.4914 (15)	C16—H16	0.9500
C5—H5A	0.9800	C17—C18	1.3949 (15)
C5—H5B	0.9800	C17—H17	0.9500
C5—H5C	0.9800	C18—C19	1.3879 (16)
C6—C7	1.5108 (15)	C19—C20	1.3901 (16)
C6—H6A	0.9900	C19—H19	0.9500
C6—H6B	0.9900	C20—H20	0.9500
C7—C12	1.3850 (15)	C21—H21A	0.9800
C7—C8	1.3946 (16)	C21—H21B	0.9800
C8—C9	1.3814 (15)	C21—H21C	0.9800
C8—H8	0.9500		
C10—O3—C13	116.79 (9)	C11—C10—C9	120.04 (10)
C18—O4—C21	116.59 (9)	C10—C11—C12	119.15 (11)
C1—N1—C2	124.87 (9)	C10—C11—H11	120.4
C1—N1—C6	117.30 (9)	C12—C11—H11	120.4
C2—N1—C6	117.78 (9)	C7—C12—C11	121.40 (11)
C4—N2—C1	121.75 (9)	C7—C12—H12	119.3
C4—N2—C14	121.65 (9)	C11—C12—H12	119.3
C1—N2—C14	116.56 (9)	O3—C13—H13A	109.5
O1—C1—N1	122.15 (11)	O3—C13—H13B	109.5
O1—C1—N2	121.67 (10)	H13A—C13—H13B	109.5
N1—C1—N2	116.18 (10)	O3—C13—H13C	109.5
O2—C2—N1	119.80 (10)	H13A—C13—H13C	109.5
O2—C2—C3	125.52 (11)	H13B—C13—H13C	109.5
N1—C2—C3	114.68 (10)	N2—C14—C15	114.07 (9)
C4—C3—C2	121.90 (11)	N2—C14—H14A	108.7
C4—C3—H3	119.0	C15—C14—H14A	108.7

supplementary materials

C2—C3—H3	119.0	N2—C14—H14B	108.7
C3—C4—N2	120.60 (10)	C15—C14—H14B	108.7
C3—C4—C5	121.37 (11)	H14A—C14—H14B	107.6
N2—C4—C5	118.03 (10)	C20—C15—C16	117.80 (10)
C4—C5—H5A	109.5	C20—C15—C14	120.46 (10)
C4—C5—H5B	109.5	C16—C15—C14	121.70 (10)
H5A—C5—H5B	109.5	C17—C16—C15	121.49 (10)
C4—C5—H5C	109.5	C17—C16—H16	119.3
H5A—C5—H5C	109.5	C15—C16—H16	119.3
H5B—C5—H5C	109.5	C16—C17—C18	119.94 (10)
N1—C6—C7	114.63 (9)	C16—C17—H17	120.0
N1—C6—H6A	108.6	C18—C17—H17	120.0
C7—C6—H6A	108.6	O4—C18—C19	124.37 (10)
N1—C6—H6B	108.6	O4—C18—C17	116.09 (10)
C7—C6—H6B	108.6	C19—C18—C17	119.54 (10)
H6A—C6—H6B	107.6	C18—C19—C20	119.54 (10)
C12—C7—C8	118.64 (10)	C18—C19—H19	120.2
C12—C7—C6	120.28 (11)	C20—C19—H19	120.2
C8—C7—C6	121.04 (10)	C15—C20—C19	121.68 (10)
C9—C8—C7	120.71 (11)	C15—C20—H20	119.2
C9—C8—H8	119.6	C19—C20—H20	119.2
C7—C8—H8	119.6	O4—C21—H21A	109.5
C8—C9—C10	120.06 (11)	O4—C21—H21B	109.5
C8—C9—H9	120.0	H21A—C21—H21B	109.5
C10—C9—H9	120.0	O4—C21—H21C	109.5
O3—C10—C11	124.45 (10)	H21A—C21—H21C	109.5
O3—C10—C9	115.51 (10)	H21B—C21—H21C	109.5
C2—N1—C1—O1	179.48 (10)	C7—C8—C9—C10	-0.49 (16)
C6—N1—C1—O1	2.11 (16)	C13—O3—C10—C11	-1.51 (15)
C2—N1—C1—N2	-0.05 (15)	C13—O3—C10—C9	178.71 (9)
C6—N1—C1—N2	-177.43 (9)	C8—C9—C10—O3	179.95 (9)
C4—N2—C1—O1	-178.01 (10)	C8—C9—C10—C11	0.15 (16)
C14—N2—C1—O1	4.12 (15)	O3—C10—C11—C12	-179.39 (10)
C4—N2—C1—N1	1.53 (15)	C9—C10—C11—C12	0.38 (16)
C14—N2—C1—N1	-176.34 (9)	C8—C7—C12—C11	0.28 (16)
C1—N1—C2—O2	179.50 (10)	C6—C7—C12—C11	177.94 (10)
C6—N1—C2—O2	-3.13 (15)	C10—C11—C12—C7	-0.60 (16)
C1—N1—C2—C3	-1.11 (15)	C4—N2—C14—C15	84.38 (13)
C6—N1—C2—C3	176.25 (9)	C1—N2—C14—C15	-97.75 (11)
O2—C2—C3—C4	-179.76 (12)	N2—C14—C15—C20	-126.06 (11)
N1—C2—C3—C4	0.89 (16)	N2—C14—C15—C16	56.27 (14)
C2—C3—C4—N2	0.48 (17)	C20—C15—C16—C17	-0.72 (16)
C2—C3—C4—C5	-179.79 (10)	C14—C15—C16—C17	177.00 (10)
C1—N2—C4—C3	-1.78 (16)	C15—C16—C17—C18	-0.11 (16)
C14—N2—C4—C3	175.98 (10)	C21—O4—C18—C19	-3.25 (15)
C1—N2—C4—C5	178.48 (10)	C21—O4—C18—C17	176.61 (10)
C14—N2—C4—C5	-3.75 (15)	C16—C17—C18—O4	-178.78 (9)
C1—N1—C6—C7	-95.32 (12)	C16—C17—C18—C19	1.09 (16)
C2—N1—C6—C7	87.11 (12)	O4—C18—C19—C20	178.63 (10)

N1—C6—C7—C12	78.75 (13)	C17—C18—C19—C20	-1.22 (16)
N1—C6—C7—C8	-103.65 (12)	C16—C15—C20—C19	0.58 (16)
C12—C7—C8—C9	0.27 (16)	C14—C15—C20—C19	-177.17 (10)
C6—C7—C8—C9	-177.37 (10)	C18—C19—C20—C15	0.38 (17)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C20—H20 \cdots O3 ⁱ	0.95	2.51	3.3627 (14)	150

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

Fig. 1

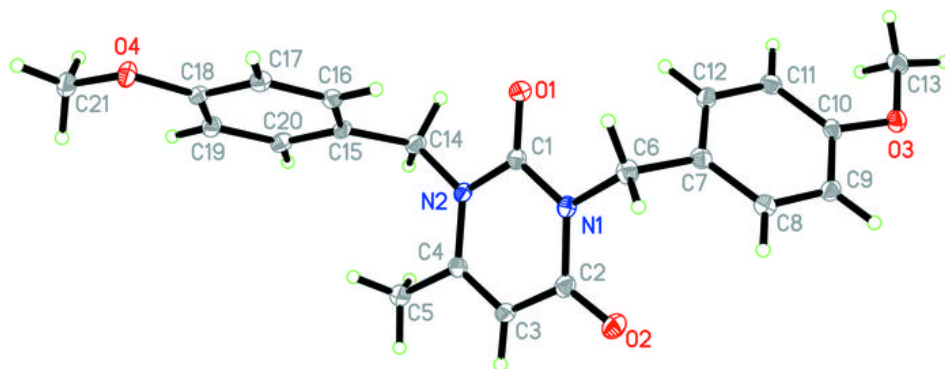


Fig. 2

