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(2*E*)-1-(3-Bromophenyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one

Jerry P. Jasinski,[a]* Ray J. Butcher,[b] C. S. Chidan Kumar,[c] H. S. Yathirajan[c] and A. N. Mayekar[d]

[a]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [b]Department of Chemistry, Howard University, 525 College Street NW, Washington DC 20059, USA, [c]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and [d]Sequent Scientif Limited, New Mangalore 57 011, India
Correspondence e-mail: jjasinski@keene.edu

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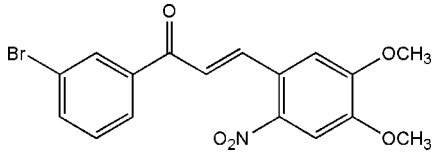
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 14.0.

In the title compound, $C_{17}H_{14}BrNO_5$, the dihedral angle between the 3-bromo-substituted benzene ring and the 4,5-dimethoxy-2-nitro-phenyl ring is 15.2 (1)°. The dihedral angles between the mean plane of the propenone group and the mean planes of the 3-bromo-substituted benzene and 4,5-dimethoxy-2-nitrophenyl rings are 6.9 (6) and 20.5 (5)°, respectively. Weak intermolecular C—H···O interactions contribute to crystal stability and π–π interactions [centroid–centroid distances = 3.7072 (18) and 3.6326 (18) Å] are also observed.

Related literature

For the biological activity of chalcones, see: Liu *et al.* (2003); Nielson *et al.* (1998); Rajas *et al.* (2002); Dinkova-Kostova *et al.* (1998). For their non-linear optical properties, see: Goto *et al.* (1991); Uchida *et al.* (1998);Tam *et al.* (1989); Indira *et al.* (2002); Sarojini *et al.* (2006). For the effect of bulky substituents on the spontaneous polarization of non-centrosymmetric crystals, see: Fichou *et al.* (1988). For the influence of the steric effect of the substituent on the molecular hyperpolarizability, see: Cho *et al.* (1996). For related structures, see: Butcher *et al.* (2007*a*,*b*,*c*); Jasinski *et al.* (2010*a*,*b*,*c*,*d*,*e*); Dutkiewicz *et al.* (2010); Kant *et al.* (2009); Yathirajan *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{14}BrNO_5$
M_r = 392.20
Orthorhombic, $P2_12_12_1$
a = 6.8547 (2) Å
b = 8.3205 (2) Å
c = 27.1509 (6) Å
V = 1548.54 (7) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.88 mm^{-1}
T = 123 K
0.55 × 0.12 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Diffractometer with Ruby Gemini detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.490, T_{max} = 1.000
9914 measured reflections
3069 independent reflections
3011 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.07
3069 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), 1228 Friedel pairs
Flack parameter: 0.08 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···O5^{i}	0.98	2.46	3.383 (3)	157
C17—H17B···O3^{ii}	0.98	2.48	3.116 (4)	123

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED*; 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: *SHELXTL*.

CSC thanks the University of Mysore for the research facilities and HSY thanks the University of Mysore for sabbatical leave. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2178).

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(2*E*)-1-(3-Bromophenyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one

Jerry P. Jasinski, Ray J. Butcher, C. S. Chidan Kumar, H. S. Yathirajan and A. N. Mayekar

S1. Comment

Chalcones have displayed an impressive array of biological activities, among which antimalarial (Liu *et al.*, 2003), antiprotozoal (Nielson *et al.*, 1998), nitric oxide inhibition (Rajas *et al.*, 2002) and anticancer activities (Dinkova-Kostova *et al.*, 1998) have been cited in the literature. Among several organic compounds reported for non-linear optical (NLO) properties, chalcone derivatives are notable materials for their excellent blue-light transmittance and good crystallizability. They provide the necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002, Sarojini *et al.*, 2006). Substitution on either of the benzene rings greatly influences the non-centrosymmetric crystal packing. It is speculated that, in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of non-centrosymmetric crystals (Fichou *et al.*, 1988). The molecular hyperpolarizability is strongly influenced, not only by the electronic effect, but also by the steric effect of the substituent (Cho *et al.*, 1996). The crystal structure studies of 2,3-dibromo-1-(2,4-dichlorophenyl)-3-(4,5-dimethoxy-2-nitrophenyl) propan-1-one (Yathirajan *et al.*, 2007); (2*E*)-1-(4-methylphenyl)-3-(4-nitrophenyl)prop-2-en-1-one (Butcher *et al.*, 2007*a*); (*E*)-3-(4-fluorophenyl)-1-(4-methylphenyl)prop-2-en-1-one (Butcher *et al.*, 2007*b*); (2*E*)-3-(2-bromo-5-methoxyphenyl)-1-(2,4-dichlorophenyl) prop-2-en-1-one (Butcher *et al.*, 2007*c*); (*E*)-3-(4-bromophenyl)-1-(3,4-dichlorophenyl)prop-2-en-1-one (Kant *et al.*, 2009); (2E)-3-(4-bromophenyl)-1-(3-chlorophenyl) prop-2-en-1-one (Jasinski *et al.*, 2010*a*); (2*E*)-1-(4-bromophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (Dutkiewicz *et al.*, 2010); (2E)-1-(2-bromophenyl)-3-(4-chlorophenyl) prop-2-en-1-one (Jasinski *et al.*, 2010*b*); (2*E*)-1-(2-bromophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Jasinski *et al.*, 2010*c*); (2*E*)-1-(2-bromophenyl)-3- (3,4,5-trimethoxyphenyl)prop-2-en-1-one (Jasinski *et al.*, 2010*d*) and (2*E*)-1-(2-bromophenyl)-3-(4-bromophenyl)prop-2-en-1-one (Jasinski *et al.*, 2010*e*) have been reported. In continuation of our work on chalcones, the present paper reports the synthesis and crystal structure of a new chalcone, $C_{17}H_{14}BrNO_5$.

In the title compound the dihedral angle between the 3-bromo-substituted benzene ring and the 4,5-dimethoxy-2-nitro-phenyl ring is 15.2 (1)° (Fig. 2). The dihedral angles between the mean plane of the propenone group and the mean planes of the 3-bromo-substituted benzene and 4,5-dimethoxy-2-nitro-phenyl rings is 6.9 (6)° and 20.5 (5)°, respectively. While no classic hydrogen bonds are observed, weak intermolecular C—H···O (Table 1, Fig. 3) hydrogen bond interactions contribute to crystal stability.

S2. Experimental

1-(3-Bromophenyl)ethanone (1.99 g, 0.01 mol) was mixed with 4,5-dimethoxy-2-nitrobenzaldehyde (2.11 g, 0.01 mol) and dissolved in methanol (30 ml). To this, 3 ml of KOH (40%) was added and the reaction mixture was stirred for 6 h (Fig. 1). The resulting crude solid was filtered, washed successively with distilled water and finally recrystallized from ethanol (95%) to give the pure chalcone. Pale yellow, small needle shaped crystals suitable for X-ray diffraction studies were grown by the slow evaporation of the dimethylformamide solution at room temperature (m.p.: 409–411 K).

S3. Refinement

The parameters of all the H atoms have been constrained within the riding atom approximation. C—H bond lengths were constrained to 0.95 or 0.98 Å for aryl or methyl H atoms, U_{iso}(H) = 1.18–1.22U_{eq}(C_{aryl}); U_{iso}(H) = 1.59–1.51U_{eq}(C_{methyl}).

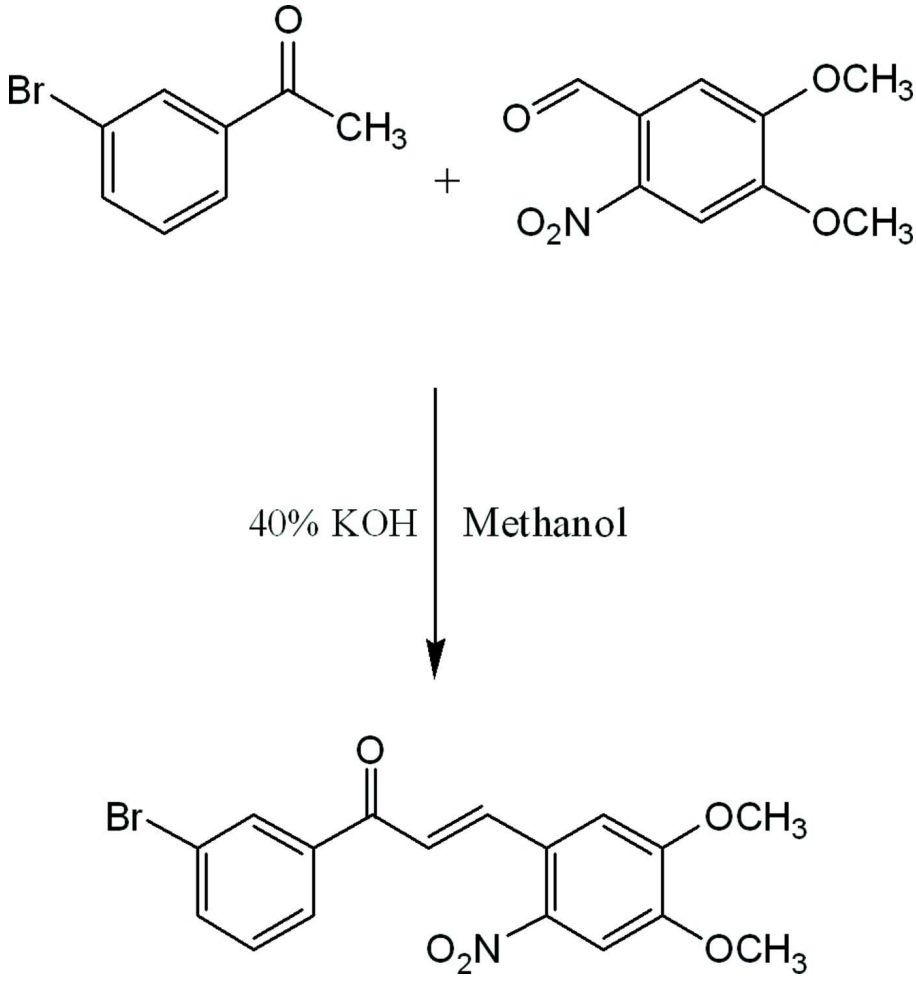

Figure 1

Reaction scheme for the title compound.

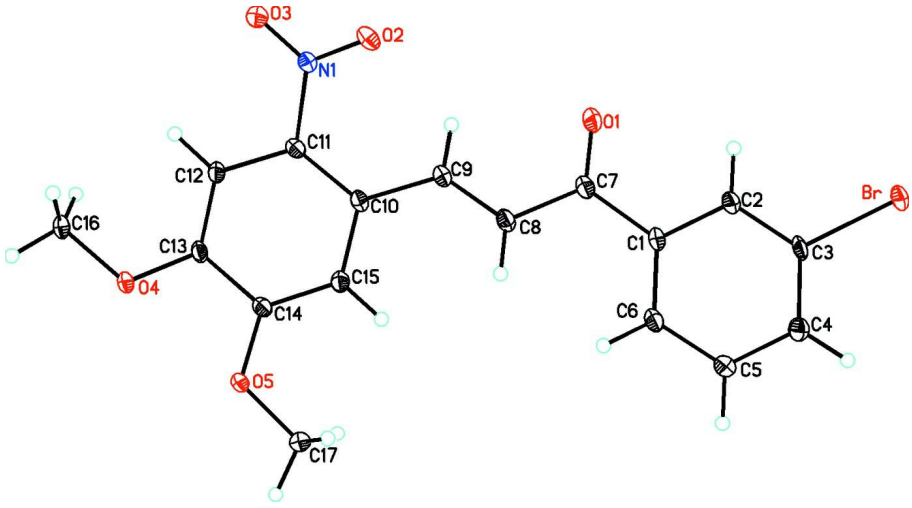

Figure 2

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

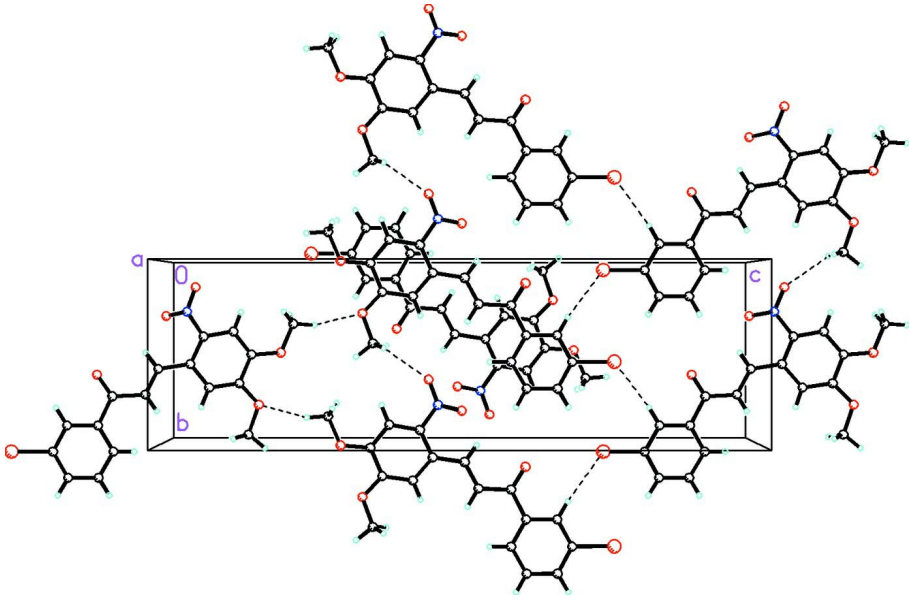

Figure 3

Packing diagram of the title compound viewed down the *a* axis. Dashed lines indicate weak intermolecular C—H···O hydrogen bond interactions.

(2*E*)-1-(3-Bromophenyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one

Crystal data

$C_{17}H_{14}BrNO_5$
M_r = 392.20
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 6.8547 (2) Å
b = 8.3205 (2) Å
c = 27.1509 (6) Å
V = 1548.54 (7) Å^3
Z = 4
F(000) = 792
D_x = 1.682 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å

Cell parameters from 8339 reflections
θ = 4.9–74.0°
μ = 3.88 mm^{-1}
T = 123 K
Needle, colorless
0.55 × 0.12 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Diffractometer with Ruby Gemini detector
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.490, T_{max} = 1.000
9914 measured reflections
3069 independent reflections
3011 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 74.1°, θ_{min} = 5.6°
h = −8→5
k = −9→10
l = −32→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.07
3069 reflections
219 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 1.5041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), 1228 Friedel pairs
Absolute structure parameter: 0.08 (2)

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}
Br	0.59396 (5)	0.54840 (4)	0.757218 (10)	0.02935 (11)
O1	0.5372 (4)	0.1224 (3)	0.60992 (8)	0.0329 (6)
O2	0.7701 (4)	−0.1958 (3)	0.50347 (8)	0.0314 (5)
O3	0.6537 (4)	−0.3581 (3)	0.44871 (9)	0.0332 (6)
O4	0.5820 (4)	0.0031 (2)	0.30190 (7)	0.0240 (4)
O5	0.5346 (4)	0.2869 (3)	0.33757 (7)	0.0258 (5)
N1	0.6855 (4)	−0.2223 (3)	0.46423 (10)	0.0227 (5)
C1	0.5862 (5)	0.4042 (3)	0.61065 (10)	0.0200 (5)
C2	0.5815 (5)	0.4043 (3)	0.66260 (10)	0.0227 (6)
H2A	0.5685	0.3064	0.6803	0.027*
C3	0.5960 (4)	0.5491 (4)	0.68724 (9)	0.0229 (5)

C4	0.6120 (5)	0.6943 (4)	0.66260 (11)	0.0247 (6)
H4A	0.6189	0.7925	0.6804	0.030*
C5	0.6179 (5)	0.6939 (4)	0.61128 (11)	0.0246 (6)
H5A	0.6296	0.7925	0.5938	0.030*
C6	0.6065 (4)	0.5491 (4)	0.58544 (10)	0.0230 (5)
H6A	0.6126	0.5494	0.5505	0.028*
C7	0.5701 (5)	0.2433 (4)	0.58575 (11)	0.0233 (6)
C8	0.5993 (5)	0.2348 (4)	0.53138 (10)	0.0224 (6)
H8A	0.6323	0.3286	0.5132	0.027*
C9	0.5783 (5)	0.0934 (3)	0.50851 (10)	0.0213 (5)
H9A	0.5488	0.0027	0.5284	0.026*
C10	0.5971 (4)	0.0665 (3)	0.45512 (9)	0.0191 (5)
C11	0.6283 (4)	−0.0843 (3)	0.43402 (10)	0.0199 (6)
C12	0.6209 (4)	−0.1121 (3)	0.38335 (10)	0.0206 (6)
H12A	0.6378	−0.2178	0.3708	0.025*
C13	0.5890 (5)	0.0144 (3)	0.35161 (9)	0.0198 (5)
C14	0.5639 (5)	0.1705 (3)	0.37128 (10)	0.0208 (6)
C15	0.5659 (4)	0.1943 (3)	0.42198 (10)	0.0203 (6)
H15A	0.5457	0.2995	0.4346	0.024*
C16	0.5963 (5)	−0.1555 (4)	0.28128 (10)	0.0255 (6)
H16A	0.5866	−0.1490	0.2453	0.038*
H16B	0.4900	−0.2223	0.2941	0.038*
H16C	0.7219	−0.2032	0.2904	0.038*
C17	0.5316 (6)	0.4499 (4)	0.35512 (11)	0.0317 (7)
H17A	0.5242	0.5236	0.3270	0.048*
H17B	0.6509	0.4714	0.3739	0.048*
H17C	0.4177	0.4657	0.3764	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.04312 (19)	0.03241 (16)	0.01252 (15)	0.00224 (15)	−0.00131 (12)	−0.00345 (11)
O1	0.0530 (16)	0.0300 (11)	0.0157 (10)	−0.0028 (11)	0.0034 (10)	−0.0018 (9)
O2	0.0428 (14)	0.0333 (12)	0.0180 (11)	0.0038 (11)	−0.0085 (10)	0.0032 (9)
O3	0.0540 (16)	0.0227 (11)	0.0228 (11)	0.0026 (10)	0.0012 (10)	0.0005 (9)
O4	0.0377 (12)	0.0219 (9)	0.0123 (8)	−0.0006 (9)	−0.0012 (9)	−0.0026 (7)
O5	0.0456 (14)	0.0191 (10)	0.0125 (9)	−0.0002 (9)	−0.0034 (9)	0.0008 (8)
N1	0.0303 (13)	0.0223 (12)	0.0154 (11)	0.0032 (10)	0.0026 (10)	0.0010 (10)
C1	0.0200 (13)	0.0264 (13)	0.0135 (12)	0.0000 (12)	−0.0016 (12)	−0.0037 (10)
C2	0.0286 (15)	0.0251 (13)	0.0145 (13)	0.0015 (13)	0.0007 (13)	−0.0009 (10)
C3	0.0288 (14)	0.0309 (14)	0.0089 (11)	0.0029 (16)	−0.0014 (11)	−0.0035 (11)
C4	0.0282 (16)	0.0251 (13)	0.0207 (14)	0.0019 (13)	0.0019 (14)	−0.0027 (11)
C5	0.0298 (16)	0.0241 (14)	0.0200 (14)	0.0004 (13)	−0.0003 (13)	0.0022 (11)
C6	0.0255 (14)	0.0285 (14)	0.0150 (12)	0.0026 (15)	−0.0007 (11)	−0.0004 (11)
C7	0.0263 (15)	0.0280 (14)	0.0158 (13)	0.0005 (13)	−0.0018 (12)	−0.0008 (11)
C8	0.0258 (14)	0.0269 (13)	0.0146 (13)	−0.0019 (14)	0.0013 (12)	0.0002 (11)
C9	0.0252 (14)	0.0243 (13)	0.0144 (12)	0.0000 (12)	0.0004 (12)	0.0002 (10)
C10	0.0207 (12)	0.0234 (13)	0.0133 (12)	−0.0023 (13)	0.0001 (11)	−0.0006 (10)

C11	0.0227 (15)	0.0214 (13)	0.0155 (13)	−0.0002 (11)	0.0002 (11)	0.0025 (10)
C12	0.0267 (16)	0.0199 (12)	0.0150 (13)	−0.0012 (12)	0.0015 (12)	−0.0037 (10)
C13	0.0250 (14)	0.0229 (13)	0.0115 (11)	−0.0017 (12)	0.0004 (11)	−0.0024 (10)
C14	0.0253 (15)	0.0213 (13)	0.0159 (13)	−0.0019 (12)	0.0010 (11)	0.0023 (11)
C15	0.0232 (15)	0.0213 (13)	0.0163 (13)	−0.0007 (11)	−0.0001 (11)	−0.0022 (10)
C16	0.0371 (16)	0.0259 (14)	0.0135 (12)	0.0011 (14)	−0.0005 (14)	−0.0053 (10)
C17	0.056 (2)	0.0186 (14)	0.0210 (14)	−0.0006 (15)	0.0011 (13)	0.0006 (13)

Geometric parameters (Å, º)

Br—C3	1.900 (3)	C7—C8	1.491 (4)
O1—C7	1.222 (4)	C8—C9	1.338 (4)
O2—N1	1.233 (4)	C8—H8A	0.9500
O3—N1	1.225 (4)	C9—C10	1.472 (4)
O4—C13	1.354 (3)	C9—H9A	0.9500
O4—C16	1.436 (3)	C10—C11	1.395 (4)
O5—C14	1.348 (4)	C10—C15	1.410 (4)
O5—C17	1.437 (4)	C11—C12	1.396 (4)
N1—C11	1.465 (4)	C12—C13	1.378 (4)
C1—C6	1.393 (4)	C12—H12A	0.9500
C1—C2	1.411 (4)	C13—C14	1.415 (4)
C1—C7	1.504 (4)	C14—C15	1.391 (4)
C2—C3	1.382 (4)	C15—H15A	0.9500
C2—H2A	0.9500	C16—H16A	0.9800
C3—C4	1.386 (4)	C16—H16B	0.9800
C4—C5	1.394 (4)	C16—H16C	0.9800
C4—H4A	0.9500	C17—H17A	0.9800
C5—C6	1.397 (4)	C17—H17B	0.9800
C5—H5A	0.9500	C17—H17C	0.9800
C6—H6A	0.9500		
C13—O4—C16	116.8 (2)	C10—C9—H9A	117.2
C14—O5—C17	117.1 (2)	C11—C10—C15	116.1 (2)
O3—N1—O2	123.1 (3)	C11—C10—C9	123.7 (3)
O3—N1—C11	118.9 (3)	C15—C10—C9	120.0 (2)
O2—N1—C11	118.0 (2)	C10—C11—C12	123.3 (3)
C6—C1—C2	119.5 (2)	C10—C11—N1	121.1 (2)
C6—C1—C7	123.8 (2)	C12—C11—N1	115.5 (2)
C2—C1—C7	116.6 (2)	C13—C12—C11	119.7 (3)
C3—C2—C1	118.9 (3)	C13—C12—H12A	120.2
C3—C2—H2A	120.6	C11—C12—H12A	120.2
C1—C2—H2A	120.6	O4—C13—C12	125.1 (2)
C2—C3—C4	122.2 (2)	O4—C13—C14	115.9 (2)
C2—C3—Br	118.8 (2)	C12—C13—C14	119.0 (2)
C4—C3—Br	119.1 (2)	O5—C14—C15	124.8 (3)
C3—C4—C5	118.9 (3)	O5—C14—C13	114.9 (2)
C3—C4—H4A	120.6	C15—C14—C13	120.2 (3)
C5—C4—H4A	120.6	C14—C15—C10	121.7 (3)

C4—C5—C6	120.2 (3)	C14—C15—H15A	119.1
C4—C5—H5A	119.9	C10—C15—H15A	119.1
C6—C5—H5A	119.9	O4—C16—H16A	109.5
C1—C6—C5	120.4 (2)	O4—C16—H16B	109.5
C1—C6—H6A	119.8	H16A—C16—H16B	109.5
C5—C6—H6A	119.8	O4—C16—H16C	109.5
O1—C7—C8	121.2 (3)	H16A—C16—H16C	109.5
O1—C7—C1	120.3 (3)	H16B—C16—H16C	109.5
C8—C7—C1	118.5 (3)	O5—C17—H17A	109.5
C9—C8—C7	119.1 (3)	O5—C17—H17B	109.5
C9—C8—H8A	120.5	H17A—C17—H17B	109.5
C7—C8—H8A	120.5	O5—C17—H17C	109.5
C8—C9—C10	125.5 (3)	H17A—C17—H17C	109.5
C8—C9—H9A	117.2	H17B—C17—H17C	109.5

C6—C1—C2—C3	0.4 (5)	C9—C10—C11—N1	−13.0 (5)
C7—C1—C2—C3	179.9 (3)	O3—N1—C11—C10	157.6 (3)
C1—C2—C3—C4	1.0 (5)	O2—N1—C11—C10	−25.0 (4)
C1—C2—C3—Br	−178.9 (3)	O3—N1—C11—C12	−26.6 (4)
C2—C3—C4—C5	−1.4 (5)	O2—N1—C11—C12	150.9 (3)
Br—C3—C4—C5	178.6 (3)	C10—C11—C12—C13	2.7 (5)
C3—C4—C5—C6	0.4 (5)	N1—C11—C12—C13	−173.1 (3)
C2—C1—C6—C5	−1.4 (5)	C16—O4—C13—C12	4.4 (5)
C7—C1—C6—C5	179.1 (3)	C16—O4—C13—C14	−176.6 (3)
C4—C5—C6—C1	1.0 (5)	C11—C12—C13—O4	178.8 (3)
C6—C1—C7—O1	−174.2 (3)	C11—C12—C13—C14	−0.2 (5)
C2—C1—C7—O1	6.3 (5)	C17—O5—C14—C15	8.8 (5)
C6—C1—C7—C8	7.0 (5)	C17—O5—C14—C13	−172.7 (3)
C2—C1—C7—C8	−172.5 (3)	O4—C13—C14—O5	0.6 (4)
O1—C7—C8—C9	3.7 (5)	C12—C13—C14—O5	179.7 (3)
C1—C7—C8—C9	−177.6 (3)	O4—C13—C14—C15	179.1 (3)
C7—C8—C9—C10	178.3 (3)	C12—C13—C14—C15	−1.8 (5)
C8—C9—C10—C11	161.5 (3)	O5—C14—C15—C10	179.9 (3)
C8—C9—C10—C15	−24.4 (5)	C13—C14—C15—C10	1.5 (5)
C15—C10—C11—C12	−2.9 (4)	C11—C10—C15—C14	0.8 (4)
C9—C10—C11—C12	171.4 (3)	C9—C10—C15—C14	−173.8 (3)
C15—C10—C11—N1	172.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*A*···O5^{i}	0.98	2.46	3.383 (3)	157
C17—H17*B*···O3^{ii}	0.98	2.48	3.116 (4)	123

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