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N,*N*′-Bis(2-acetylphenyl)ethanediamide, a second polymorph

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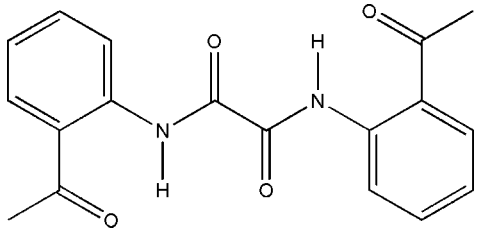
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.113; data-to-parameter ratio = 15.2.

Two new polymorphs of *N*,*N*′-bis(2-acetylphenyl)ethanediamide, $C_{18}H_{16}N_2O_4$, are reported, one crystallizing in the space group $P\overline{1}$, in the present paper, and one in $P2_1/n$ [Brewer, Jasinski, Butcher & Scheidt (2007). *Acta Cryst.* E**63**, o4887–o4888]. In both structures, the 2-acetyl group is twisted slightly away from the plane of the benzene ring. In the present paper, this polymorph crystallizes with two half-molecules (*A* and *B*) in the asymmetric unit, each of which lies on an inversion center located at the centroid of an ethanediamide unit. The molecules adopt *trans* ethanediamide (oxanalide) configurations, whereby the amide H atoms are bifurcated intramolecular hydrogen-bonding donors to oxamine and acetyl O atoms. The crystal packing is stabilized by intermolecular C—H···O hydrogen-bond interactions.

Related literature

For the synthesis of the title compound, see: Black *et al.* (1982); Black & Moss (1987). For the $P2_1/n$ polymorph and related references, see: Brewer *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{16}N_2O_4$
M_r = 324.33
Triclinic, $P\overline{1}$
a = 3.9567 (4) Å
b = 12.3429 (12) Å
c = 15.3884 (15) Å
α = 87.622 (2)°
β = 83.998 (2)°
γ = 86.662 (2)°
V = 745.66 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 170 K
0.38 × 0.15 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4585 measured reflections
3228 independent reflections
2471 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.113
S = 0.96
3228 reflections
213 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1*A*—H1*AA*···O2*A*	0.88	1.95	2.6377 (15)	134
N1*A*—H1*AA*···O1*A*^{i}	0.88	2.24	2.6709 (16)	110
N1*B*—H1*BA*···O2*B*	0.88	1.92	2.6408 (15)	137
N1*B*—H1*BA*···O1*B*^{ii}	0.88	2.24	2.6741 (15)	110
C9*A*—H9*B*···O1*B*^{iii}	0.98	2.44	3.3717 (18)	159

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2431).

References

Black, D., Bos Vanderzalm, C. H. & Wong, L. C. H. (1982). *Aust. J. Chem.* **35**, 2435–2443.
Black, D. & Moss, G. I. (1987). *Aust. J. Chem.* **40**, 129–42.
Brewer, G., Jasinski, J. P., Butcher, R. J. & Scheidt, W. R. (2007). *Acta Cryst.* E**63**, 4887–4888..
Bruker (2000). *SMART* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). *SAINT*. Bruker AXS Inc., Madison Wisconsin, USA.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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N,*N*'-Bis(2-acetylphenyl)ethanediamide, a second polymorph

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Comment

Two new polymorphs of the type $C_{18}H_{16}N_2O_4$ are reported, one which crystalizes in the spacegroup P 2_1/n (I), and one crystallizing in spacegroup P −1 (II), as reported in the present paper. For the structure of the polymorph in P 2_1/n and related references, see Brewer *et al.* (2007). In the present paper the molecule crystallizes with two half molecules (A & B) in the asymmetric unit (Fig. 1) each of which lies about an inversion centre located at the centroid of an ethanediamide unit. The 2-acetyl group of each molecule is twisted slightly away from the plane of the phenyl ring as evidenced by their respective torsion angles [C1A–C2A–C8A–C9A (175.20 (12)°) and C1B–C2B–C8B–C9B (179.63 (13)°)]. Each molecule adopts a *trans* ethanediamide (oxanilide) conformation, whereby, the amide hydrogen atoms are bifurcated intramolecular hydrogen bonding donors to oxamide and acetyl oxygen atoms [N1A—H1AA··· O1A^{i}, N1B—H1BA···O1B^{ii}; i = −*x* + 2, −*y*, −*z* + 1, ii = −*x* + 1, −*y* + 1, −*z*]. Crystal packing is stabilized by intermolecular C9A—H9B···OB hydrogen bond interactions [−*x* + 1, −*y*, −*z*] (Fig.2). In spite of crystallizing in different space groups [(I) in P 2_1/n, (II) in P −1] both compounds are nearly isostructural.

Experimental

The title molecule was synthesized by the condensation of oxalyl chloride and 2-aminoacetophenone as described previously (Black *et al.*, 1982, 1987). The resulting solid was recrystallized from *N*,*N*-dimethylformamide (DMF) and gave two polymorphs, orange-brown irregular bocks [P 2_1/n, (I)] and colorless needles [P −1. (II)] which were analyzed by *x*-ray diffraction.

Refinement

The amide hydrogen atoms (H1AA & H1BA) were located in a difference Fourier map and along with all other H atoms were placed in their calculated positions and then refined using the riding model with N—H = 0.88 Å; C—H = 0.95 to 0.98 Å, and U_{iso}(H) = 1.19–1.49U_{eq}(C,*N*).

Figures

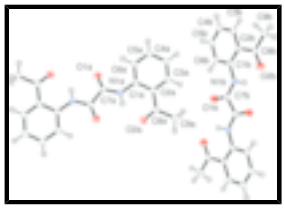

Fig. 1. Molecular structure of molecules A & B for (II), showing atom labeling and 50% probability displacement ellipsoids. Labeled atoms are related to unlabeled atoms by the symmetry operations −*x* + 2, −*y*, −*z* + 1 for A and −*x* + 1, −*y* + 1, −*z* for B.

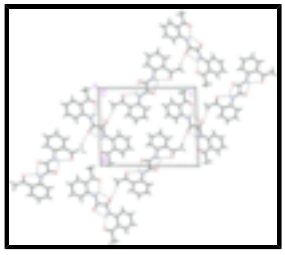

Fig. 2. Packing diagram of (II), viewed down the *a* axis. Dashed lines indicate C–H···O intermolecular and N–H···O intramolecular hydrogen bonds.

N,*N*'-bis(2-acetylphenyl)ethanediamide

Crystal data

$C_{18}H_{16}N_2O_4$	$Z = 2$
$M_r = 324.33$	$F_{000} = 340$
Triclinic, $P\overline{1}$	$D_x = 1.445$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 3.9567$ (4) Å	Cell parameters from 2785 reflections
$b = 12.3429$ (12) Å	$\theta = 2.7$–28.3º
$c = 15.3884$ (15) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 87.622$ (2)º	$T = 170$ K
$\beta = 83.998$ (2)º	Needle, colorless
$\gamma = 86.662$ (2)º	0.38 × 0.15 × 0.05 mm
$V = 745.66$ (13) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2471 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.013$
Monochromator: graphite	$\theta_{max} = 28.3$º
$T = 170$ K	$\theta_{min} = 2.2$º
φ and ω scans	$h = -4 \rightarrow 5$
Absorption correction: none	$k = -16 \rightarrow 13$
4585 measured reflections	$l = -16 \rightarrow 20$
3228 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.113$	$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{max} = <0.001$
3228 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}

213 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1A	0.7120 (3)	0.07092 (8)	0.57413 (6)	0.0328 (3)
N1A	0.8884 (3)	0.11120 (9)	0.42932 (7)	0.0249 (3)
H1AA	1.0223	0.0849	0.3850	0.030*
C1A	0.7094 (3)	0.21000 (11)	0.41266 (9)	0.0242 (3)
O2A	1.0252 (3)	0.10196 (9)	0.25823 (6)	0.0354 (3)
C2A	0.6857 (3)	0.24688 (11)	0.32485 (9)	0.0244 (3)
C3A	0.5110 (4)	0.34693 (12)	0.30995 (9)	0.0289 (3)
H3A	0.4933	0.3727	0.2515	0.035*
C4A	0.3639 (2)	0.40902 (7)	0.37780 (5)	0.0321 (3)
H4A	0.2463	0.4765	0.3661	0.039*
C5A	0.3898 (2)	0.37150 (7)	0.46396 (5)	0.0310 (3)
H5A	0.2895	0.4137	0.5111	0.037*
C6A	0.5607 (2)	0.27338 (7)	0.48077 (5)	0.0279 (3)
H6A	0.5772	0.2487	0.5396	0.034*
C7A	0.8809 (3)	0.05137 (11)	0.50501 (9)	0.0244 (3)
C8A	0.8436 (4)	0.18464 (12)	0.24842 (9)	0.0264 (3)
C9A	0.7829 (4)	0.22522 (12)	0.15771 (9)	0.0307 (3)
H9A	0.8985	0.1751	0.1151	0.046*
H9B	0.8725	0.2974	0.1468	0.046*
H9C	0.5380	0.2296	0.1521	0.046*
O1B	0.2442 (3)	0.43801 (9)	0.08505 (7)	0.0385 (3)
N1B	0.4038 (3)	0.61469 (9)	0.06662 (7)	0.0246 (3)
H1BA	0.5165	0.6576	0.0282	0.030*
C1B	0.2566 (3)	0.66347 (11)	0.14349 (8)	0.0228 (3)
O2B	0.6584 (3)	0.80449 (8)	0.02183 (6)	0.0351 (3)
C2B	0.3204 (3)	0.77333 (11)	0.15688 (8)	0.0229 (3)
C3B	0.1813 (4)	0.81964 (12)	0.23501 (9)	0.0266 (3)
H23A	0.2273	0.8924	0.2454	0.032*
C4B	−0.0206 (4)	0.76275 (12)	0.29725 (9)	0.0297 (3)
H24A	−0.1133	0.7960	0.3497	0.036*

C5B	−0.0867 (4)	0.65670 (12)	0.28242 (9)	0.0292 (3)
H25A	−0.2287	0.6175	0.3247	0.035*
C6B	0.0514 (4)	0.60665 (11)	0.20665 (9)	0.0260 (3)
H26A	0.0058	0.5334	0.1978	0.031*
C7B	0.3944 (4)	0.51058 (11)	0.04421 (9)	0.0255 (3)
C8B	0.5298 (4)	0.84046 (11)	0.09129 (9)	0.0252 (3)
C9B	0.5825 (4)	0.95662 (11)	0.11071 (10)	0.0303 (3)
H29A	0.7378	0.9882	0.0639	0.045*
H29B	0.6806	0.9589	0.1665	0.045*
H29C	0.3634	0.9983	0.1144	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0447 (6)	0.0285 (6)	0.0234 (5)	0.0031 (5)	0.0024 (4)	−0.0001 (4)
N1A	0.0323 (7)	0.0213 (6)	0.0204 (6)	0.0017 (5)	−0.0009 (5)	−0.0001 (5)
C1A	0.0266 (7)	0.0202 (7)	0.0260 (7)	−0.0036 (6)	−0.0020 (6)	−0.0006 (5)
O2A	0.0487 (7)	0.0289 (6)	0.0268 (6)	0.0084 (5)	−0.0011 (5)	−0.0016 (4)
C2A	0.0258 (7)	0.0228 (7)	0.0250 (7)	−0.0049 (6)	−0.0031 (5)	0.0006 (6)
C3A	0.0325 (8)	0.0264 (8)	0.0278 (8)	−0.0012 (6)	−0.0046 (6)	0.0026 (6)
C4A	0.0347 (8)	0.0225 (8)	0.0385 (9)	0.0041 (6)	−0.0043 (6)	0.0004 (6)
C5A	0.0355 (8)	0.0268 (8)	0.0300 (8)	0.0004 (6)	0.0010 (6)	−0.0052 (6)
C6A	0.0336 (8)	0.0254 (8)	0.0247 (7)	−0.0025 (6)	−0.0019 (6)	−0.0015 (6)
C7A	0.0301 (8)	0.0217 (7)	0.0222 (7)	−0.0036 (6)	−0.0044 (6)	−0.0019 (5)
C8A	0.0294 (8)	0.0236 (8)	0.0262 (7)	−0.0064 (6)	−0.0013 (6)	−0.0002 (6)
C9A	0.0383 (9)	0.0302 (8)	0.0235 (7)	−0.0039 (7)	−0.0016 (6)	0.0009 (6)
O1B	0.0564 (7)	0.0228 (6)	0.0343 (6)	−0.0084 (5)	0.0101 (5)	−0.0037 (4)
N1B	0.0346 (7)	0.0185 (6)	0.0201 (6)	−0.0015 (5)	−0.0002 (5)	−0.0007 (4)
C1B	0.0264 (7)	0.0224 (7)	0.0200 (6)	0.0033 (5)	−0.0062 (5)	−0.0011 (5)
O2B	0.0512 (7)	0.0254 (6)	0.0276 (5)	−0.0055 (5)	0.0049 (5)	−0.0037 (4)
C2B	0.0265 (7)	0.0208 (7)	0.0219 (7)	0.0021 (5)	−0.0062 (5)	−0.0011 (5)
C3B	0.0317 (8)	0.0246 (8)	0.0243 (7)	0.0024 (6)	−0.0066 (6)	−0.0054 (6)
C4B	0.0332 (8)	0.0336 (8)	0.0220 (7)	0.0040 (6)	−0.0030 (6)	−0.0058 (6)
C5B	0.0306 (8)	0.0321 (8)	0.0239 (7)	0.0017 (6)	−0.0017 (6)	0.0027 (6)
C6B	0.0299 (7)	0.0227 (7)	0.0255 (7)	−0.0001 (6)	−0.0048 (6)	0.0007 (6)
C7B	0.0316 (8)	0.0215 (7)	0.0232 (7)	0.0002 (6)	−0.0032 (6)	−0.0010 (6)
C8B	0.0301 (8)	0.0229 (7)	0.0230 (7)	0.0020 (6)	−0.0058 (6)	−0.0015 (6)
C9B	0.0365 (8)	0.0219 (8)	0.0328 (8)	−0.0012 (6)	−0.0047 (6)	−0.0019 (6)

Geometric parameters (Å, °)

O1A—C7A	1.2204 (16)	O1B—C7B	1.2197 (17)
N1A—C7A	1.3517 (17)	N1B—C7B	1.3478 (18)
N1A—C1A	1.4021 (18)	N1B—C1B	1.4054 (17)
N1A—H1AA	0.8800	N1B—H1BA	0.8800
C1A—C6A	1.3936 (16)	C1B—C6B	1.3931 (19)
C1A—C2A	1.4186 (18)	C1B—C2B	1.4207 (19)
O2A—C8A	1.2269 (18)	O2B—C8B	1.2240 (16)
C2A—C3A	1.402 (2)	C2B—C3B	1.3990 (18)

C2A—C8A	1.4930 (19)	C2B—C8B	1.4925 (19)
C3A—C4A	1.3797 (17)	C3B—C4B	1.378 (2)
C3A—H3A	0.9500	C3B—H23A	0.9500
C4A—C5A	1.3982	C4B—C5B	1.382 (2)
C4A—H4A	0.9500	C4B—H24A	0.9500
C5A—C6A	1.3806	C5B—C6B	1.3882 (19)
C5A—H5A	0.9500	C5B—H25A	0.9500
C6A—H6A	0.9500	C6B—H26A	0.9500
C7A—C7A^{i}	1.539 (3)	C7B—C7B^{ii}	1.544 (3)
C8A—C9A	1.5016 (19)	C8B—C9B	1.5072 (19)
C9A—H9A	0.9800	C9B—H29A	0.9800
C9A—H9B	0.9800	C9B—H29B	0.9800
C9A—H9C	0.9800	C9B—H29C	0.9800
C7A—N1A—C1A	128.06 (11)	C7B—N1B—C1B	128.27 (11)
C7A—N1A—H1AA	116.0	C7B—N1B—H1BA	115.9
C1A—N1A—H1AA	116.0	C1B—N1B—H1BA	115.9
C6A—C1A—N1A	121.15 (11)	C6B—C1B—N1B	121.60 (12)
C6A—C1A—C2A	119.59 (12)	C6B—C1B—C2B	119.45 (12)
N1A—C1A—C2A	119.24 (12)	N1B—C1B—C2B	118.95 (12)
C3A—C2A—C1A	118.14 (13)	C3B—C2B—C1B	118.27 (12)
C3A—C2A—C8A	119.09 (12)	C3B—C2B—C8B	119.09 (12)
C1A—C2A—C8A	122.76 (12)	C1B—C2B—C8B	122.64 (12)
C4A—C3A—C2A	121.87 (13)	C4B—C3B—C2B	121.88 (13)
C4A—C3A—H3A	119.1	C4B—C3B—H23A	119.1
C2A—C3A—H3A	119.1	C2B—C3B—H23A	119.1
C3A—C4A—C5A	119.25 (7)	C3B—C4B—C5B	119.18 (13)
C3A—C4A—H4A	120.4	C3B—C4B—H24A	120.4
C5A—C4A—H4A	120.4	C5B—C4B—H24A	120.4
C6A—C5A—C4A	120.3	C4B—C5B—C6B	120.97 (13)
C6A—C5A—H5A	119.9	C4B—C5B—H25A	119.5
C4A—C5A—H5A	119.9	C6B—C5B—H25A	119.5
C5A—C6A—C1A	120.89 (7)	C5B—C6B—C1B	120.22 (13)
C5A—C6A—H6A	119.6	C5B—C6B—H26A	119.9
C1A—C6A—H6A	119.6	C1B—C6B—H26A	119.9
O1A—C7A—N1A	127.46 (13)	O1B—C7B—N1B	127.51 (12)
O1A—C7A—C7A^{i}	121.43 (15)	O1B—C7B—C7B^{ii}	120.97 (15)
N1A—C7A—C7A^{i}	111.11 (14)	N1B—C7B—C7B^{ii}	111.52 (14)
O2A—C8A—C2A	121.33 (13)	O2B—C8B—C2B	122.12 (12)
O2A—C8A—C9A	119.44 (13)	O2B—C8B—C9B	118.82 (12)
C2A—C8A—C9A	119.22 (13)	C2B—C8B—C9B	119.06 (12)
C8A—C9A—H9A	109.5	C8B—C9B—H29A	109.5
C8A—C9A—H9B	109.5	C8B—C9B—H29B	109.5
H9A—C9A—H9B	109.5	H29A—C9B—H29B	109.5
C8A—C9A—H9C	109.5	C8B—C9B—H29C	109.5
H9A—C9A—H9C	109.5	H29A—C9B—H29C	109.5
H9B—C9A—H9C	109.5	H29B—C9B—H29C	109.5
C7A—N1A—C1A—C6A	16.6 (2)	C7B—N1B—C1B—C6B	−4.7 (2)
C7A—N1A—C1A—C2A	−164.68 (13)	C7B—N1B—C1B—C2B	175.15 (14)

C6A—C1A—C2A—C3A	−0.09 (19)	C6B—C1B—C2B—C3B	1.9 (2)
N1A—C1A—C2A—C3A	−178.79 (12)	N1B—C1B—C2B—C3B	−177.93 (12)
C6A—C1A—C2A—C8A	178.86 (11)	C6B—C1B—C2B—C8B	−178.34 (13)
N1A—C1A—C2A—C8A	0.16 (19)	N1B—C1B—C2B—C8B	1.8 (2)
C1A—C2A—C3A—C4A	−0.1 (2)	C1B—C2B—C3B—C4B	−1.7 (2)
C8A—C2A—C3A—C4A	−179.05 (11)	C8B—C2B—C3B—C4B	178.48 (13)
C2A—C3A—C4A—C5A	0.12 (16)	C2B—C3B—C4B—C5B	0.3 (2)
C3A—C4A—C5A—C6A	−0.03 (8)	C3B—C4B—C5B—C6B	1.0 (2)
C4A—C5A—C6A—C1A	−0.12 (7)	C4B—C5B—C6B—C1B	−0.8 (2)
N1A—C1A—C6A—C5A	178.86 (8)	N1B—C1B—C6B—C5B	179.16 (12)
C2A—C1A—C6A—C5A	0.19 (14)	C2B—C1B—C6B—C5B	−0.7 (2)
C1A—N1A—C7A—O1A	1.1 (2)	C1B—N1B—C7B—O1B	3.0 (3)
C1A—N1A—C7A—C7A^{i}	−179.51 (13)	C1B—N1B—C7B—C7B^{ii}	−177.01 (14)
C3A—C2A—C8A—O2A	173.14 (13)	C3B—C2B—C8B—O2B	179.92 (13)
C1A—C2A—C8A—O2A	−5.8 (2)	C1B—C2B—C8B—O2B	0.1 (2)
C3A—C2A—C8A—C9A	−5.86 (18)	C3B—C2B—C8B—C9B	−0.6 (2)
C1A—C2A—C8A—C9A	175.20 (12)	C1B—C2B—C8B—C9B	179.63 (13)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1A—H1AA···O2A	0.88	1.95	2.6377 (15)	134
N1A—H1AA···O1A^{i}	0.88	2.24	2.6709 (16)	110
N1B—H1BA···O2B	0.88	1.92	2.6408 (15)	137
N1B—H1BA···O1B^{ii}	0.88	2.24	2.6741 (15)	110
C9A—H9B···O1B^{iii}	0.98	2.44	3.3717 (18)	159

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

Fig. 1

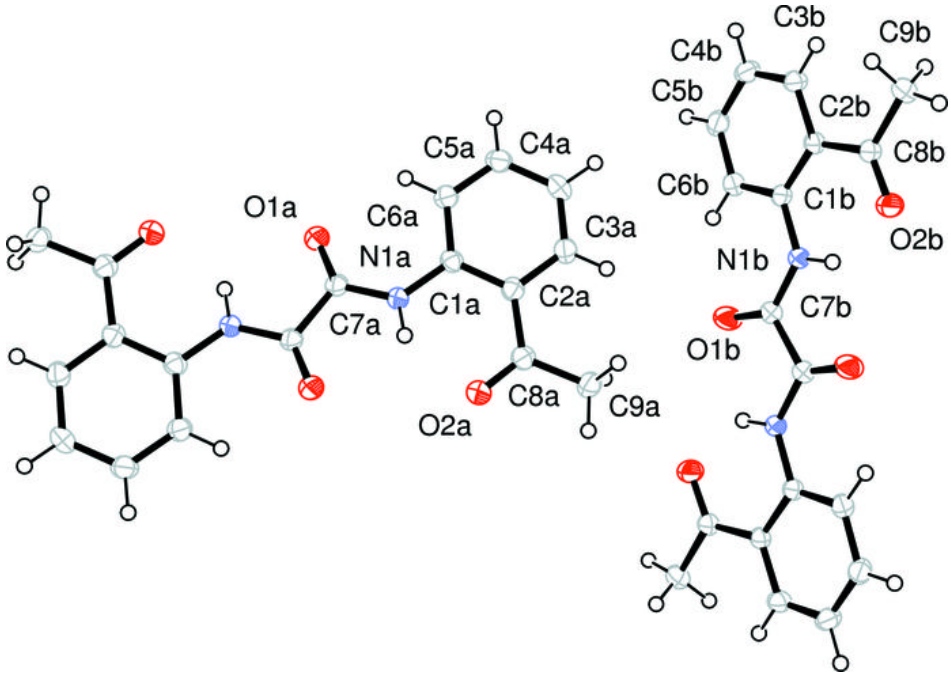
C3b
C9b
C4b
C5b
C2b
C8b
C6b
C1b
O2b
N1b
C7b
O1b
C5a
C4a
O1a
C6a
C3a
N1a
C1a
C2a
C7a
C8a
C9a
O2a

Fig. 2