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(*RS*/*SR*)-2-Oxo-4-phenylazetidin-3-yl acetate

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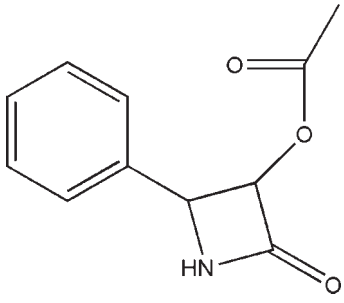
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.125; data-to-parameter ratio = 8.2.

In the title compound, $C_{11}H_{11}NO_3$, a modified synthetic acetate derivative, the four memebered β-lactam ring is roughly planar, with a maximum deviation of 0.21 (3) Å, and makes a dihedral angle of 81.46 (14)° with the phenyl ring. In the crystal, a single N—H···O hydrogen bond links molecules into a chain parallel to the a axis and thus stabilizes the structure. Although the absolute configuration could not be reliably determined, the compound corresponds to the diasteroisomer (*RS*/*SR*)

Related literature

For properties of lactams, see: Selvanayagam *et al.* (2005); Deschamps *et al.* (2003); Kanazawa *et al.* (1993). For a related structure, see: Akkurt *et al.* (2007).



Experimental

Crystal data

$C_{11}H_{11}NO_3$
M_r = 205.21
Orthorhombic, $P2_12_12_1$
a = 5.940 (4) Å
b = 8.198 (4) Å
c = 20.896 (13) Å
V = 1017.6 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.21 × 0.16 × 0.10 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.980, T_{max} = 0.990
1899 measured reflections
1126 independent reflections
853 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
S = 1.17
1126 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.11	2.943 (3)	162

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{5}{2}, -z+2$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* ; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2490).

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supporting information

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(*RS*/*SR*)-2-Oxo-4-phenylazetidin-3-yl acetate

Yangjun Li

S1. Comment

Recently, lactams have attracted much attention because they are convenient intermediates for semi-synthesis of the antitumour drug Taxol and other bioactive analogues (Kanazawa *et al.*, 1993). Furthermore, the lactam ring (azetidin-2-one) is considered a general 'lead structure′ for the design of new inhibitors of enzymes containing a serine nucleophile in the active site (Deschamps *et al.*, 2003). In an attempt to form a Zn(II) complex with title compound, we adventitiously formed the title compound (I) and its crystal structure is determined herein.

The molecular structure of (I) is illustrated in Fig. 1. It is very similar to the related 4-(4-Nitrophenyl)-3-phenoxy-azetidin-2-one (Akkurt *et al.*, 2007). The geometry of the *β*-lactam ring is is planar, with a maximum deviation of 0.21 (3)° for atom N1. It makes dihedral angles of 81.46 (14)° with its phenyl substituent. The lactam ting is also comparable with a related reported structure (Selvanayagam *et al.*, 2005). Although the absolute configuration couldn't be reliably determined, the compound correspond to the diasteroisomer (RS/SR).

Intermolecular N-H···O hydrogen bonds form a zig-zag like chain parallel to the a axis and thus stabilize the structure. (Table 1, Figure 2).

S2. Experimental

The title compound was obtained by direct mixing of equimolar (28mg, 0.1mmol) $Zn(OAC)_2.6H_2O$ of water solution (8mL) and 2-Oxo-4-phenylazetidin-3-yl acetate (21mg, 0.1mmol), and CH_3CN and CH_3CH_2OH solutions (5mL). using slow evaporation of the solvent at room temperature over a period of about two weeks.

S3. Refinement

In the absence of significant anomalous scattering, the absolute configuration could not be reliably determined and then the Friedel pairs were merged and any references to the Flack parameter were removed.

All H atoms were placed in calculated positions (C-H = 0.93 (aromatic), N-H=0.86, or 0.96 Å (methyl)) refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$(aromatic), $U_{iso}(H) = 1.5U_{eq}(C)$ (methyl).

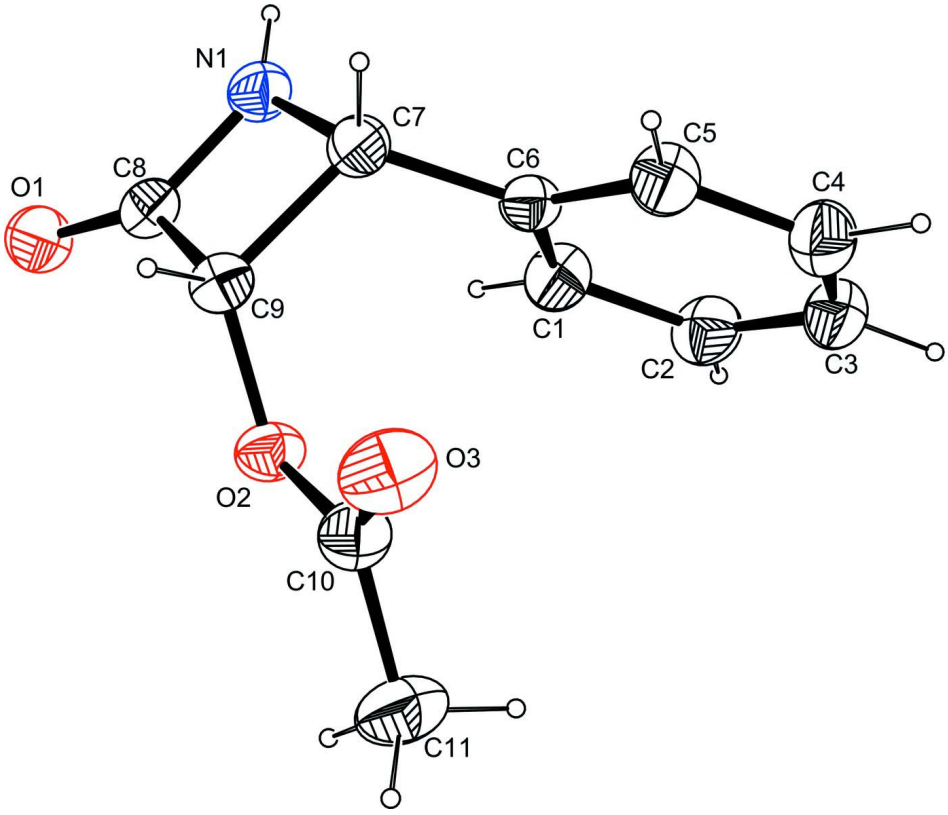

Figure 1

Molecular view of (I) with the atom-labeling scheme. Ellipsoids are drawn at the the 30% probability level. H atoms are shown as spheres of arbitrary radii.

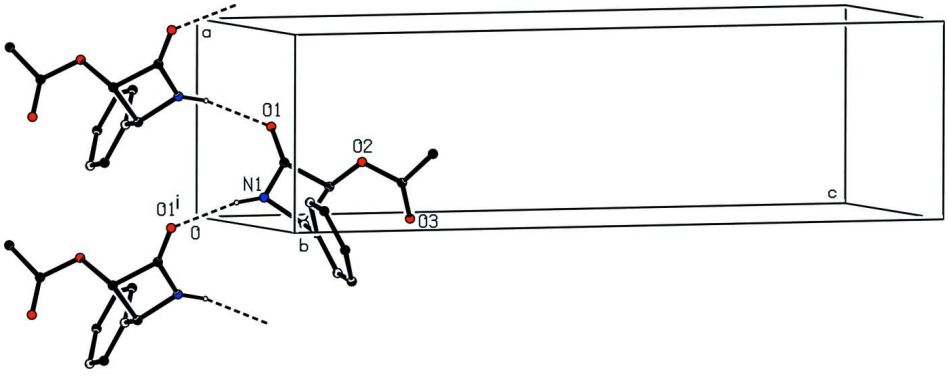

Figure 2

Partial packing view showing the formation of the chain parallel to the a axis. H atoms not involved in hydrogen bondings have been omitted for clarity. [Symmetry code: (i) x-1/2, -y+5/2, -z+2]

(*RS*/*SR*)-2-Oxo-4-phenylazetidin-3-yl acetate

Crystal data

$C_{11}H_{11}NO_3$
M_r = 205.21
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 5.940 (4) Å
b = 8.198 (4) Å

c = 20.896 (13) Å
V = 1017.6 (11) Å^3
Z = 4
F(000) = 432
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 1899 reflections
θ = 2.0–25.5°
μ = 0.10 mm^{-1}
T = 298 K
Block, colorless
0.21 × 0.16 × 0.10 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.980, T_{max} = 0.990

1899 measured reflections
1126 independent reflections
853 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.5°, θ_{min} = 2.0°
h = −7→7
k = 0→9
l = −25→0

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
S = 1.17
1126 reflections
137 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
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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 > 2sigma(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	0.6268 (6)	0.7783 (4)	0.93447 (16)	0.0536 (9)
H1	0.7589	0.8249	0.9498	0.064*
C2	0.5969 (7)	0.6098 (4)	0.93779 (16)	0.0598 (10)
H2	0.7093	0.5443	0.9551	0.072*
C3	0.4038 (7)	0.5413 (4)	0.91576 (16)	0.0613 (10)
H3	0.3853	0.4288	0.9176	0.074*
C4	0.2362 (7)	0.6368 (4)	0.89092 (16)	0.0624 (10)
H4	0.1036	0.5894	0.8763	0.075*
C5	0.2647 (6)	0.8040 (4)	0.88758 (14)	0.0543 (9)
H5	0.1502	0.8688	0.8710	0.065*

C6	0.4617 (5)	0.8759 (4)	0.90866 (13)	0.0412 (7)
C7	0.4897 (6)	1.0577 (3)	0.90075 (14)	0.0449 (7)
H7	0.3451	1.1122	0.8935	0.054*
C8	0.7926 (6)	1.1852 (3)	0.91243 (13)	0.0434 (7)
C9	0.6733 (5)	1.1182 (3)	0.85319 (13)	0.0418 (7)
H9	0.6188	1.2043	0.8246	0.050*
C10	0.7031 (7)	0.9236 (4)	0.77046 (14)	0.0523 (9)
C11	0.8572 (7)	0.7982 (4)	0.74195 (15)	0.0747 (12)
H11A	0.8191	0.6924	0.7584	0.112*
H11B	1.0101	0.8237	0.7530	0.112*
H11C	0.8409	0.7984	0.6962	0.112*
N1	0.6232 (5)	1.1404 (3)	0.95028 (11)	0.0480 (7)
H1A	0.5996	1.1550	0.9905	0.058*
O1	0.9694 (4)	1.2566 (3)	0.92206 (9)	0.0555 (6)
O2	0.8050 (4)	0.9987 (2)	0.82088 (8)	0.0468 (6)
O3	0.5181 (5)	0.9564 (3)	0.75310 (12)	0.0712 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.048 (2)	0.0518 (18)	0.0607 (19)	0.0040 (16)	−0.0083 (17)	−0.0020 (16)
C2	0.067 (3)	0.0467 (18)	0.065 (2)	0.0129 (18)	−0.001 (2)	0.0082 (16)
C3	0.072 (3)	0.0455 (17)	0.066 (2)	−0.0057 (19)	0.009 (2)	−0.0021 (16)
C4	0.057 (2)	0.0561 (19)	0.074 (2)	−0.0084 (18)	−0.003 (2)	−0.0076 (17)
C5	0.050 (2)	0.0534 (18)	0.0593 (19)	0.0017 (17)	−0.0051 (17)	−0.0001 (15)
C6	0.0416 (19)	0.0429 (14)	0.0391 (14)	0.0017 (15)	0.0034 (14)	−0.0025 (12)
C7	0.0427 (19)	0.0433 (15)	0.0486 (15)	0.0005 (15)	0.0000 (15)	−0.0026 (12)
C8	0.049 (2)	0.0366 (14)	0.0448 (16)	0.0036 (15)	−0.0017 (16)	−0.0025 (12)
C9	0.0434 (19)	0.0418 (13)	0.0403 (14)	0.0038 (15)	−0.0018 (14)	−0.0026 (13)
C10	0.061 (2)	0.0573 (18)	0.0385 (15)	−0.0031 (18)	−0.0030 (16)	−0.0029 (13)
C11	0.073 (3)	0.083 (2)	0.068 (2)	0.009 (2)	−0.002 (2)	−0.030 (2)
N1	0.0590 (18)	0.0466 (13)	0.0383 (12)	−0.0024 (13)	0.0040 (13)	−0.0064 (11)
O1	0.0506 (15)	0.0620 (13)	0.0540 (12)	−0.0106 (12)	−0.0019 (11)	−0.0112 (10)
O2	0.0450 (13)	0.0540 (11)	0.0415 (11)	0.0019 (12)	−0.0005 (9)	−0.0109 (9)
O3	0.0721 (18)	0.0842 (16)	0.0572 (12)	0.0093 (16)	−0.0186 (13)	−0.0125 (12)

Geometric parameters (Å, º)

C1—C6	1.376 (4)	C7—H7	0.9800
C1—C2	1.395 (4)	C8—O1	1.219 (4)
C1—H1	0.9300	C8—N1	1.332 (4)
C2—C3	1.357 (5)	C8—C9	1.529 (4)
C2—H2	0.9300	C9—O2	1.424 (3)
C3—C4	1.369 (5)	C9—H9	0.9800
C3—H3	0.9300	C10—O3	1.188 (4)
C4—C5	1.383 (4)	C10—O2	1.362 (4)
C4—H4	0.9300	C10—C11	1.500 (5)
C5—C6	1.382 (4)	C11—H11A	0.9600

C5—H5	0.9300	C11—H11B	0.9600
C6—C7	1.509 (4)	C11—H11C	0.9600
C7—N1	1.469 (4)	N1—H1A	0.8600
C7—C9	1.556 (4)		

C6—C1—C2	120.3 (4)	C9—C7—H7	111.8
C6—C1—H1	119.8	O1—C8—N1	133.3 (3)
C2—C1—H1	119.8	O1—C8—C9	134.9 (3)
C3—C2—C1	120.0 (4)	N1—C8—C9	91.8 (2)
C3—C2—H2	120.0	O2—C9—C8	112.1 (2)
C1—C2—H2	120.0	O2—C9—C7	117.9 (2)
C2—C3—C4	120.4 (3)	C8—C9—C7	85.5 (2)
C2—C3—H3	119.8	O2—C9—H9	112.8
C4—C3—H3	119.8	C8—C9—H9	112.8
C3—C4—C5	119.8 (4)	C7—C9—H9	112.8
C3—C4—H4	120.1	O3—C10—O2	123.0 (3)
C5—C4—H4	120.1	O3—C10—C11	126.7 (3)
C6—C5—C4	120.7 (3)	O2—C10—C11	110.2 (3)
C6—C5—H5	119.7	C10—C11—H11A	109.5
C4—C5—H5	119.7	C10—C11—H11B	109.5
C1—C6—C5	118.7 (3)	H11A—C11—H11B	109.5
C1—C6—C7	122.6 (3)	C10—C11—H11C	109.5
C5—C6—C7	118.7 (3)	H11A—C11—H11C	109.5
N1—C7—C6	116.0 (3)	H11B—C11—H11C	109.5
N1—C7—C9	85.7 (2)	C8—N1—C7	96.7 (2)
C6—C7—C9	117.5 (2)	C8—N1—H1A	131.6
N1—C7—H7	111.8	C7—N1—H1A	131.6
C6—C7—H7	111.8	C10—O2—C9	115.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.86	2.11	2.943 (3)	162

Symmetry code: (i) $x-1/2, -y+5/2, -z+2$.