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Isopropyl 2-oxo-3,4-dihydro-1,4-benzoxazine-4-acetate

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In the crystal structure of the title compound, $C_{13}H_{15}NO_4$, adjacent molecules are linked together by C—H···O hydrogen bonding to form one-dimensional supramolecular chains.

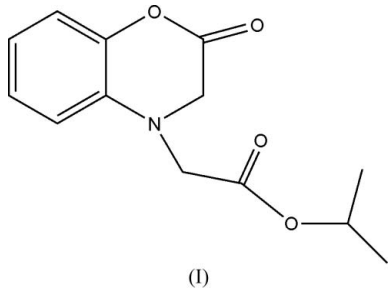
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.057
wR factor = 0.274
Data-to-parameter ratio = 13.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

We have an interest in aminoacetic acid and its derivatives because of their applications in pesticides, medicine and food additives (Wang, 2004). We recently prepared the title compound, (I), and determined its crystal structure.



(I)

The molecular structure of (I) is shown in Fig. 1. C—H···O hydrogen bonding (Table 1) helps to stabilize the crystal structure of (I) (Fig. 2).

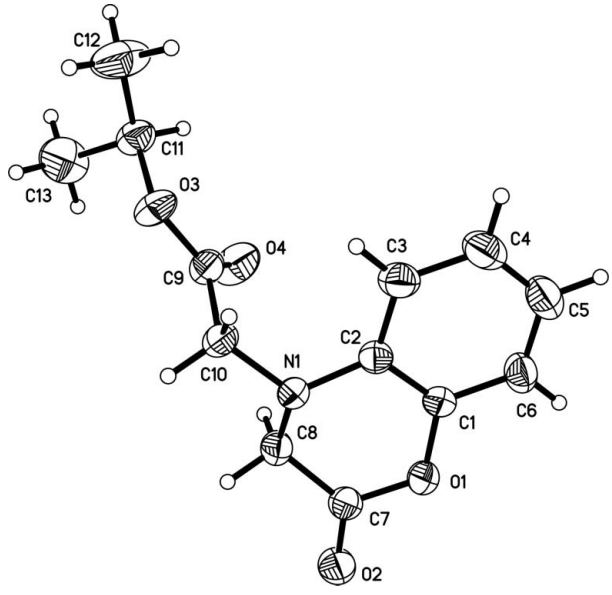


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Experimental

3,4-Dihydro-1,4-benzoxazin-2-one-4-acetic acid (0.146 g, 0.5 mmol) was added to isopropyl alcohol (15 ml) in a Teflon-lined stainless steel reactor. The mixture was heated at 413 K for 3 d. After cooling to room temperature colorless single crystals of (I) were obtained; yield 0.560 g (69%).

Crystal data

$C_{13}H_{15}NO_4$
M_r = 249.26
Monoclinic, $P2_1/c$
a = 13.632 (6) Å
b = 9.587 (4) Å
c = 10.240 (5) Å
β = 108.349 (6)°
V = 1270.2 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.48 × 0.39 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
6376 measured reflections
2234 independent reflections
1134 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.274
S = 1.00
2234 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2^{i}	0.93	2.63	3.531 (5)	163
C8—H8B···O1^{ii}	0.97	2.62	3.443 (5)	143
C10—H10B···O2^{ii}	0.97	2.60	3.483 (5)	151

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

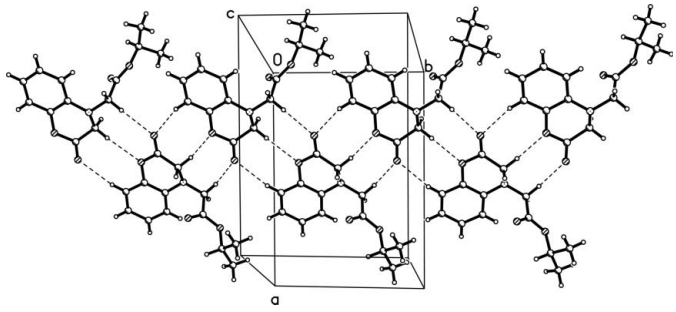


Figure 2
The packing of (I), showing C—H···O hydrogen bonding (dashed lines).

All H atoms were placed geometrically and treated as riding on their parent atoms, with C—H = 0.93 (aromatic), 0.97 (methylene), 0.96 (methyl) and 0.98 Å (methine). The U_{iso}(H) values were set as $1.5U_{eq}$(C) for methyl groups and $1.2U_{eq}$(C) for the other H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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