organic papers

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Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.170
Data-to-parameter ratio = 13.2

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

Methyl 2-(methoxyacetylamino)benzoate

The title compound, $C_{11}H_{13}NO_4$, was obtained by reaction of methyl 2-aminobenzoate and 2-methoxyacetyl chloride. The two side chains lie in the same plane as the benzene ring.

Comment

Methyl 2-(methoxyacetylamino)benzoate, (I), is an important intermediate in the chemical industry (Aavid *et al.*, 1949) and is used extensively in medicine and pesticides (Stephen *et al.*, 2002). For example, it is a precursor of quinazoline derivatives and a potential anticancer medication (Silvana *et al.*, 2004). We report here the synthesis and crystal structure of the title compound, (I). The two side chains lie in the same plane as the benzene ring plane (dihedral angle 1.4°).
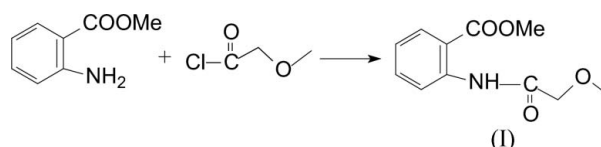
Experimental

2-Methoxyacetyl chloride (5.38 g, 0.05 mol) was added dropwise over a period of 30 min to a dichloromethane (60 ml) solution of methyl 2-aminobenzoate (5.00 g, 0.033 mol) and pyridine (5.22 g, 0.066 mol) in a cool water bath (273–278 K), then the mixture was stirred for 2 h at room temperature. The resulting solution was washed with $1M$ HCl (50 ml), 1 M NaOH (50 ml), saturated NaCl (50 ml) and water (50 ml). The dichloromethane solution was dried over $MgSO_4$, and the solvent was removed using a rotary evaporator to give (I) as a white solid (yield: 4.80 g, 65%; m.p. 345–346 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a CH_2Cl_2 solution at room temperature. Analysis calculated for $C_{11}H_{13}NO_4$: C 59.19, H 5.87, N 6.28, O 28.67%; found: C 59.33, H 5.54, N 6.44, O 28.76%.

Crystal data

$C_{11}H_{13}NO_4$	$V = 555.8$ (5) Å^3
$M_r = 223.22$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.334$ Mg m^{-3}
$a = 7.149$ (4) Å	Mo $K\alpha$ radiation
$b = 8.649$ (5) Å	$\mu = 0.10$ mm^{-1}
$c = 9.973$ (5) Å	$T = 293$ (2) K
$\alpha = 67.462$ (5)°	Prism, colorless
$\beta = 89.982$ (7)°	$0.24 \times 0.16 \times 0.12$ mm
$\gamma = 78.350$ (7)°	

Data collection

Bruker SMART CCD area-detector diffractometer	3000 measured reflections
φ and ω scans	1941 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1166 reflections with $I > 2\sigma(I)$
$T_{min} = 0.975$, $T_{max} = 0.988$	$R_{int} = 0.029$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0937P)^2]$
$wR(F^2) = 0.170$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
1941 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
147 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}

All H atoms were initially located in a difference Fourier map, but were then constrained to an ideal geometry, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and refined as riding on their parent atoms.

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

Figure 1
A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

References

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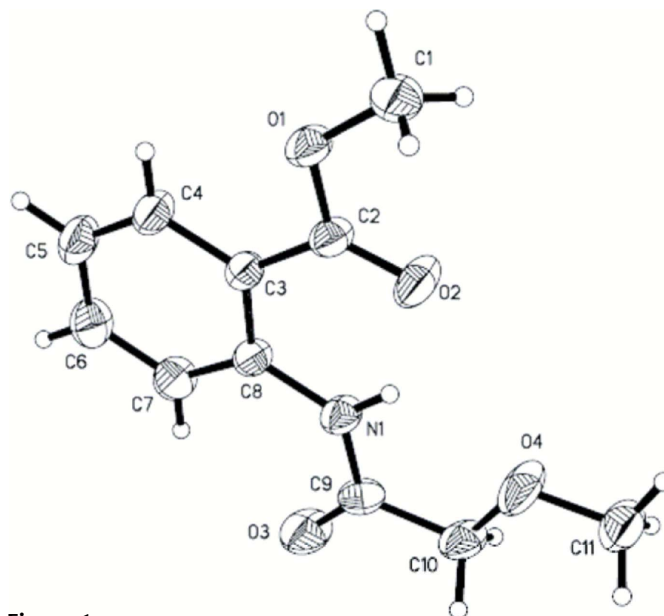Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
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