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N-(2-Acetyl-3,5-dimethoxyphenyl)acetamide

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Key indicators

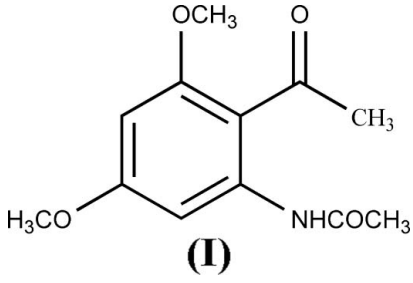
Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.095
Data-to-parameter ratio = 14.8

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

In the title compound, $C_{12}H_{15}NO_4$, the molecular packing is influenced by inter- and intramolecular C—H···O hydrogen bonds. The two methoxy groups are almost in the same plane, and the acetamide group is somewhat twisted out of the benzene ring plane.

Comment

4-Quinolones are a group of synthetic antimicrobial agents that exhibit excellent potential and a broad spectrum of activity against a variety of bacteria (Mitscher, 2005). In addition, they are commonly used as antitumour agents (Xia *et al.*, 2003). In this paper, we present the X-ray crystallographic analysis of the title compound, (I), which is an important intermediate for the synthesis of 4-quinolones.



(I)

In the title structure (Fig. 1), the bond lengths and angles are in good agreement with the expected values (Allen *et al.*,

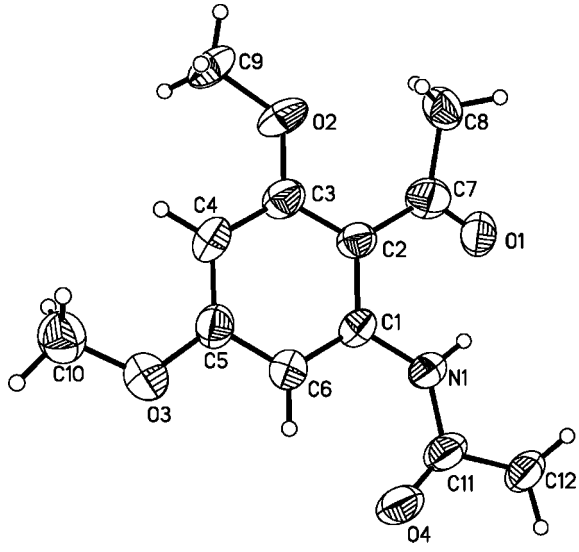


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

1987). The dihedral angle between the acetamide group and benzene ring is 4.5 (5)°.

In the packing of (I), the molecules are linked by intermolecular hydrogen bonds (Table 1, Fig. 2), thereby stabilizing the crystal structure.

Experimental

To a solution of 3,5-dimethoxyacetanilide (0.1952 g, 1 mmol) in dry 1,2-dichloroethane (5 ml) at 273 K, anhydrous stannic chloride (0.234 ml, 2 mmol) was added. Acetyl chloride (0.156 ml, 2.2 mmol) was then added dropwise and the reaction mixture was stirred for 3 h. After the reaction was complete, the mixture was poured into ice–water, extracted with CH_2Cl_2 (30 ml), washed with saturated $NaHCO_3$ solution and brine, and dried over anhydrous Na_2SO_4. The solvent was evaporated *in vacuo* and the residue was separated by column chromatography (petroleum ether–ethyl acetate 5:1 *v*/*v*) to give the product (m.p. 382 K). Single crystals of (I) were obtained by slow evaporation of a petroleum ether–ethyl acetate (5:1 *v*/*v*) solution of (I).

Crystal data

$C_{12}H_{15}NO_4$
M_r = 237.25
Monoclinic, $P2_1/c$
a = 7.166 (3) Å
b = 17.156 (8) Å
c = 10.181 (5) Å
β = 107.059 (6)°
V = 1196.6 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.98
6381 measured reflections
2347 independent reflections
1406 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.095
S = 0.98
2347 reflections
159 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.9	2.612 (3)	139
C6—H6···O4	0.93	2.20	2.830 (3)	125
C12—H12A···O4^{i}	0.96	2.54	3.487 (3)	169

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

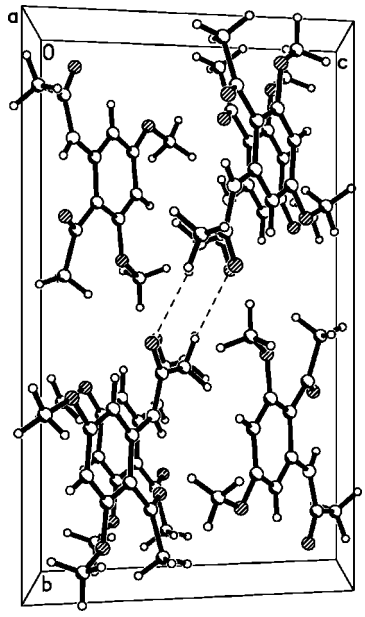


Figure 2
A packing diagram for (I), viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93–0.96 Å or N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(C) for methyl H.

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

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2000). *SMART*, *SAINT-Plus*, *SHELXTL* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Mitscher, L. A. (2005). *Chem. Rev.* **105**, 559–592.
Xia, Y., Yang, Z. Y., Xia, P., Bastow, K. F., Nakanishi, Y., Nampoothiri, P., Hamel, E., Brossia, A. & Lee, K.-H. (2003). *Bioorg. Med. Chem. Lett.* **13**, 2891–2893.