Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Acetylphenyl)maleamic acid

Daniel E. Lynch[a]* and Ian McClenaghan[b]

[a]School of Science and the Environment, Coventry University, Coventry CV1 5FB, England, and [b]Key Organics Ltd, Highfield Industrial Estate, Camelford, Cornwall PL32 9QZ, England

Correspondence e-mail: apx106@coventry.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.133
Data-to-parameter ratio = 13.7

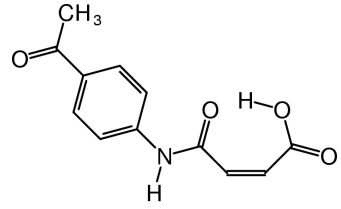
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 May 2002
Accepted 16 May 2002
Online 24 May 2002

The structure of the title compound, $C_{12}H_{11}NO_4$, comprises an essentially flat molecule displaying a typical maleic acid intramolecular hydrogen bond. An intermolecular N—H···O association exists from the amide to the carboxylic acid carbonyl O atom, while several C—H···O close contacts are observed around the maleamic acid O atoms.

Comment

The structure of the title compound, (I), comprises an essentially flat molecule displaying a typical maleic acid intramolecular hydrogen bond. In this interaction, the O···O distance of 2.465 (2) Å is short, whereas the refined O—H distance of 1.11 (3) Å is longer than expected. The corresponding H···O distance of 1.37 (3) Å indicates that the H atom is essentially delocalized between the two O atoms. An intermolecular N—H···O association exists from the amide to the carboxylic acid carbonyl O atom, while several C—H···O close contacts are observed around the maleamic acid O atoms. The title compound is a precursor to the corresponding maleimide.



(I)

Experimental

The title compound was obtained from Key Organics Ltd. Crystals were grown from an ethanol solution.

Crystal data

$C_{12}H_{11}NO_4$
M_r = 233.22
Monoclinic, $P2_1/c$
a = 5.5577 (3) Å
b = 25.5016 (14) Å
c = 7.4588 (5) Å
β = 95.134 (2)°
V = 1052.90 (11) Å^3
Z = 4
D_x = 1.471 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6037 reflections
θ = 1.0–27.5°
μ = 0.11 mm^{-1}
T = 150 (2) K
Block, yellow
0.10 × 0.10 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.989, T_{max} = 0.989
5131 measured reflections
2227 independent reflections
1479 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°
$h = -7 \rightarrow 7$
$k = -32 \rightarrow 33$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.133$
$S = 1.05$
2227 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.0474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···O10^{i}	0.88 (2)	1.93 (2)	2.809 (2)	178 (2)
O11—H11···O81	1.11 (3)	1.37 (3)	2.465 (2)	169 (2)
C2—H2···O81	0.95	2.24	2.842 (2)	121
C6—H6···O10^{i}	0.95	2.54	3.289 (2)	136
C9—H9···O11^{i}	0.95	2.59	3.533 (2)	174

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

All H atoms were included in the refinement, at calculated positions, as riding models, with C—H set to 0.95 (Ar—H) and 0.98 Å (CH_3), except for the carboxylic acid and amine H atoms, which were located in a difference synthesis; these atoms were refined freely.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

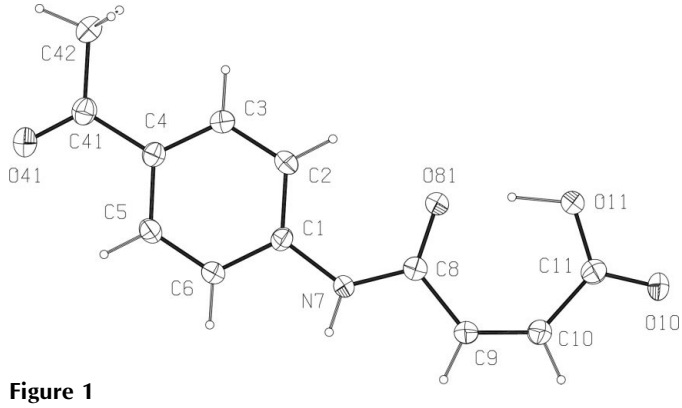


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 50% probability ellipsoids.

The authors thank the EPSRC National Crystallography Service (Southampton).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1997). *PLATON*97. Version of May 1997. University of Utrecht, The Netherlands.