Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(*p*-Tolyl)maleamic acid

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Received 20 June 2002
Accepted 8 July 2002
Online 19 July 2002

Key indicators

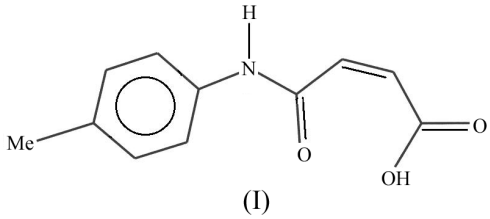
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.177
Data-to-parameter ratio = 12.3

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

The title molecule, $C_{11}H_{11}NO_3$, is nearly planar, with the mean planes through the *p*-tolyl and maleamic acid groups inclined at an angle of 5.45 (3)°. The glide-related molecules are linked by N—H···O and C—H···O intermolecular hydrogen bonds, forming infinite one-dimensional chains, which are assembled to form layers parallel to the *bc* plane.

Comment

The structure of *N*-(*p*-tolyl)maleamic acid, (I), was reported previously by Prasad & Sinha (1978), using photographic X-ray diffraction data, with an R value of 0.16. The structure has now been refined using single-crystal X-ray diffraction data and the results are presented here.



(I)

The molecule of (I) is nearly planar, with C3 deviating by a maximum of 0.103 (3) Å. The mean planes through the *p*-tolyl and maleamic acid groups are inclined at an angle of 5.45 (3)° (Table 1). The bond lengths and angles in the maleamic acid group agree with those reported for the structure of maleic acid (James & Williams, 1974). The carboxyl H atom is involved in an intramolecular O—H···O hydrogen bond with carbonyl atom O3. In the solid state, the glide-related molecules are linked by N—H···O and C—H···O hydrogen bonds (Table 2), forming infinite one-dimensional chains along the *c*-cell direction. These chains are arranged so as to form layers parallel to the *bc* plane, approximately at x = 1/4 and 3/4. The mean interlayer separation of 3.406 Å indicates significant interactions between the aryl and maleamic acid groups; the shortest interlayer contacts are C6···C10($-x$, $1-y$, $1-z$) of 3.319 (5) Å and C4···C7($1-x$, $1-y$, $1-z$) of 3.351 (4) Å.

Experimental

The title compound was prepared by a solid-state reaction between *p*-phenylaniline and maleic anhydride by Professor R. P. Rastogi (Gorakhpur University) and his co-workers (private communication) and was recrystallized from methanol at room temperature.

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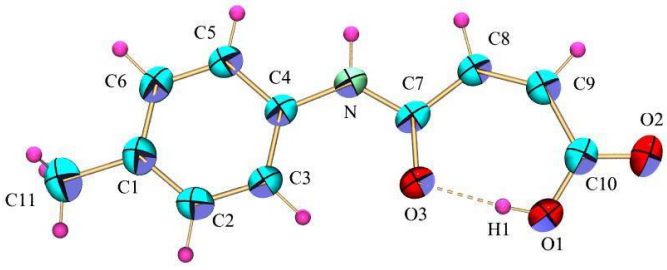

Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

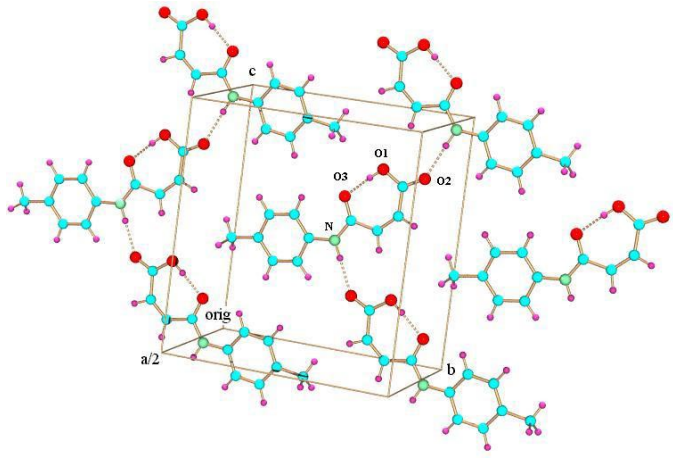

Figure 2
A view of the molecular layer, close to x = 1/4.

Crystal data

$C_{11}H_{11}NO_3$
M_r = 205.21
Monoclinic, $P2_1/c$
a = 6.769 (2) Å
b = 12.109 (1) Å
c = 12.606 (1) Å
β = 95.73 (1)°
V = 1028.1 (3) Å^3
Z = 4
D_x = 1.326 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 28.2–36.3°
μ = 0.81 mm^{-1}
T = 293 (2) K
Block, colourless
0.38 × 0.31 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.733, T_{max} = 0.817
2123 measured reflections
2047 independent reflections
1200 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 75.5°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 15$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.178
S = 1.04
2047 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 0.2017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0101 (16)

Table 1
Selected geometric parameters (Å, °).

C4—N	1.412 (3)	C8—C9	1.337 (3)
C7—O3	1.240 (3)	C10—O2	1.214 (3)
C7—N	1.343 (3)	C10—O1	1.298 (3)
C7—C8	1.467 (4)		
C3—C4—N	124.3 (2)	C9—C8—C7	128.6 (2)
C5—C4—N	116.9 (2)	C8—C9—C10	132.6 (2)
N—C7—C8	113.5 (2)	C7—N—C4	128.9 (2)
O3—C7—N—C4	0.7 (5)	C3—C4—N—C7	−6.6 (5)
C8—C7—N—C4	−179.1 (3)	C5—C4—N—C7	174.3 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N—H1N···O2^{i}	0.93 (3)	1.96 (3)	2.885 (3)	177 (2)
O1—H1O···O3	0.82	1.68	2.495 (2)	173
C3—H3···O3	0.98 (3)	2.26 (2)	2.866 (3)	119 (2)
C8—H8···O1^{i}	0.97 (3)	2.55 (2)	3.498 (3)	164 (2)

Symmetry code: (i) $x, \frac{3}{2} - y, z - \frac{1}{2}$.

All H atoms apart from the methyl and hydroxyl H atoms were refined isotropically.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

The authors acknowledge Professor R. P. Rastogi, Department of Chemistry, Gorakhpur University, for the gift of the crystals and the National Centre for X-ray Diffraction Facility, All India Institute of Medical Sciences, New Delhi, for the collection of the X-ray diffraction data.

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