Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Phenylmaleamic acid

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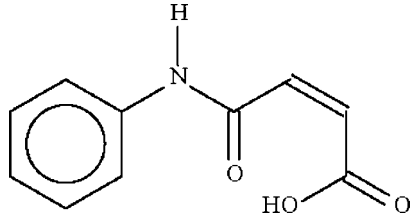
Received 18 April 2009; accepted 20 April 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.068; wR factor = 0.208; data-to-parameter ratio = 14.6.

The two independent molecules in the title compound (systematic name: 4-amino-4-oxobut-2-enoic acid), $C_{10}H_9NO_3$, are both essentially planar (r.m.s. deviations = 0.05 and 0.06 Å). In both molecules, the –OH group forms an intramolecular hydrogen bond to the amide O atom. Adjacent molecules are linked by N—H···O hydrogen bonds into a flat ribbon that runs along the *a* axis of the monoclinic unit cell.

Related literature

For the crystal structures of other substituted *N*-(phenyl)maleamic acids, see, for example: Gonzalez-Rodriguez *et al.* (1986); Home *et al.* (1991); Lynch & McClenaghan (2002); Parvez *et al.* (2004*a*,*b*); Prasad *et al.* (2002*a*,*b*); Santos-Sánchez *et al.* (2007); Wardell *et al.* (2005).



Experimental

Crystal data

$C_{10}H_9NO_3$
M_r = 191.18
Monoclinic, $P2_1/c$
a = 12.7505 (4) Å
b = 10.5849 (5) Å
c = 14.1918 (6) Å
β = 116.299 (3)°
V = 1717.1 (1) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.24 × 0.06 × 0.06 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
11493 measured reflections
3925 independent reflections
2256 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.208
S = 1.02
3925 reflections
269 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2o···O3	0.85 (1)	1.63 (1)	2.475 (3)	172 (4)
O5—H5o···O6	0.86 (1)	1.65 (1)	2.496 (3)	170 (3)
N1—H1n···O4	0.88 (1)	2.00 (1)	2.864 (3)	166 (3)
N2—H2n···O1^{i}	0.89 (1)	1.99 (1)	2.859 (3)	167 (3)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya (FS339/2008 A) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2436).

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supporting information

Acta Cryst. (2009). E**65**, o1101 [doi:10.1107/S1600536809014627]

N-Phenylmaleamic acid

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S1. Experimental

Maleic anhydride (1 g, 1 mmol) and aniline (1 ml, 1 mmol) was heated in toluene (50 ml) for 1 h. The solution was set aside for the formation of crystals.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The oxygen- and nitrogen-bound hydrogen atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 Å and N–H 0.88±0.01 Å; the temperature factors were refined.

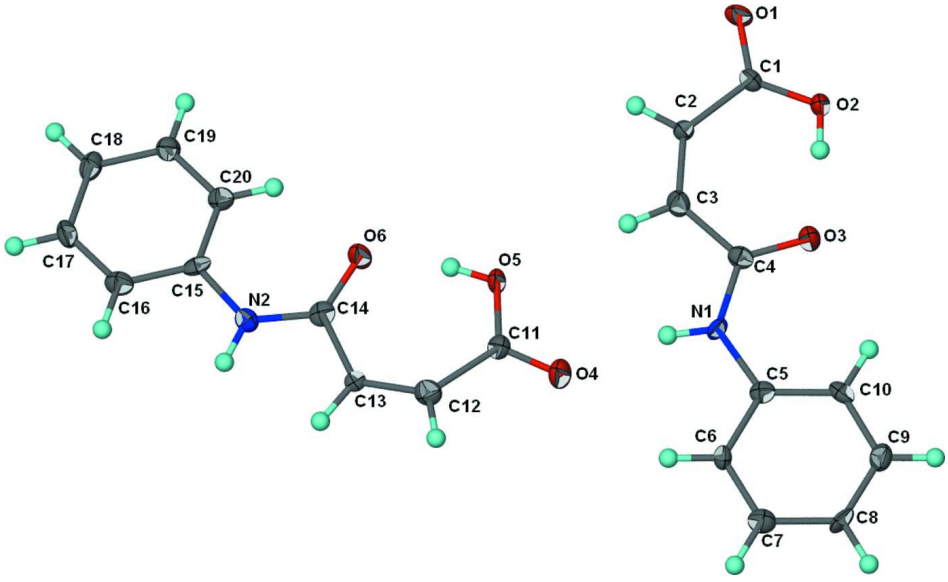

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of $C_{10}H_9NO_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

4-amino-4-oxobut-2-enoic acid

Crystal data

$C_{10}H_9NO_3$
M_r = 191.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 12.7505 (4) Å
b = 10.5849 (5) Å
c = 14.1918 (6) Å
β = 116.299 (3)°

V = 1717.1 (1) Å^3
Z = 8
F(000) = 800
D_x = 1.479 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1202 reflections

θ = 2.6–27.4°
μ = 0.11 mm^{-1}
T = 100 K
Prism, colorless
0.24 × 0.06 × 0.06 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
11493 measured reflections
3925 independent reflections

2256 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −16→16
k = −13→13
l = −14→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.208
S = 1.02
3925 reflections
269 parameters
4 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1139P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.41604 (16)	0.86211 (19)	0.61750 (16)	0.0173 (5)
O2	0.41080 (17)	0.6545 (2)	0.62972 (17)	0.0167 (5)
H2O	0.449 (3)	0.590 (3)	0.627 (3)	0.058 (14)*
O3	0.53761 (17)	0.4779 (2)	0.62899 (16)	0.0187 (5)
O4	0.91395 (17)	0.5468 (2)	0.60999 (17)	0.0216 (5)
O5	0.91031 (17)	0.75293 (19)	0.62870 (17)	0.0164 (5)
H5O	0.946 (3)	0.820 (2)	0.625 (3)	0.028 (10)*
O6	1.03470 (16)	0.93320 (19)	0.62520 (16)	0.0187 (5)
N1	0.7136 (2)	0.4490 (2)	0.62704 (18)	0.0122 (5)
H1N	0.771 (2)	0.492 (3)	0.623 (2)	0.019 (8)*
N2	1.2093 (2)	0.9624 (2)	0.62037 (19)	0.0149 (6)
H2N	1.2657 (19)	0.923 (3)	0.611 (2)	0.020 (8)*
C1	0.4591 (2)	0.7584 (3)	0.6178 (2)	0.0123 (6)
C2	0.5691 (2)	0.7538 (3)	0.6046 (2)	0.0109 (6)
H2	0.5933	0.8336	0.5906	0.013*
C3	0.6396 (2)	0.6584 (3)	0.6087 (2)	0.0157 (6)
H3	0.7079	0.6811	0.6018	0.019*
C4	0.6250 (2)	0.5224 (3)	0.6227 (2)	0.0135 (6)
C5	0.7229 (2)	0.3155 (3)	0.6348 (2)	0.0130 (6)
C6	0.8169 (2)	0.2612 (3)	0.6232 (2)	0.0118 (6)

H6	0.8710	0.3139	0.6125	0.014*
C7	0.8311 (2)	0.1321 (3)	0.6272 (2)	0.0164 (6)
H7	0.8945	0.0957	0.6188	0.020*
C8	0.7521 (2)	0.0547 (3)	0.6436 (2)	0.0149 (6)
H8	0.7609	−0.0345	0.6450	0.018*
C9	0.6615 (2)	0.1075 (3)	0.6576 (2)	0.0171 (6)
H9	0.6086	0.0544	0.6697	0.020*
C10	0.6463 (2)	0.2388 (3)	0.6541 (2)	0.0136 (6)
H10	0.5843	0.2749	0.6648	0.016*
C11	0.9577 (2)	0.6509 (3)	0.6128 (2)	0.0145 (6)
C12	1.0671 (2)	0.6566 (3)	0.5988 (2)	0.0171 (6)
H12	1.0910	0.5773	0.5836	0.021*
C13	1.1380 (2)	0.7531 (3)	0.6038 (2)	0.0095 (6)
H13	1.2070	0.7313	0.5977	0.011*
C14	1.1215 (2)	0.8896 (3)	0.6177 (2)	0.0140 (6)
C15	1.2203 (2)	1.0966 (3)	0.6289 (2)	0.0130 (6)
C16	1.3130 (2)	1.1490 (3)	0.6154 (2)	0.0169 (7)
H16	1.3645	1.0961	0.6012	0.020*
C17	1.3298 (2)	1.2781 (3)	0.6228 (2)	0.0163 (6)
H17	1.3934	1.3136	0.6143	0.020*
C18	1.2542 (2)	1.3569 (3)	0.6427 (2)	0.0165 (6)
H18	1.2659	1.4458	0.6471	0.020*
C19	1.1619 (2)	1.3044 (3)	0.6560 (2)	0.0147 (6)
H19	1.1097	1.3576	0.6689	0.018*
C20	1.1457 (2)	1.1746 (3)	0.6504 (2)	0.0147 (6)
H20	1.0835	1.1388	0.6612	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0154 (10)	0.0149 (12)	0.0241 (12)	0.0036 (8)	0.0111 (9)	−0.0025 (9)
O2	0.0143 (10)	0.0118 (12)	0.0283 (12)	0.0004 (9)	0.0133 (9)	0.0026 (9)
O3	0.0165 (10)	0.0144 (12)	0.0298 (12)	−0.0003 (8)	0.0145 (9)	0.0015 (9)
O4	0.0195 (10)	0.0149 (12)	0.0335 (13)	−0.0042 (9)	0.0145 (10)	−0.0003 (9)
O5	0.0150 (10)	0.0108 (12)	0.0280 (13)	−0.0026 (8)	0.0138 (9)	0.0000 (9)
O6	0.0176 (10)	0.0126 (12)	0.0322 (13)	−0.0003 (9)	0.0166 (9)	−0.0029 (9)
N1	0.0159 (12)	0.0072 (13)	0.0159 (12)	−0.0001 (10)	0.0091 (10)	0.0012 (10)
N2	0.0145 (12)	0.0157 (14)	0.0175 (13)	0.0013 (10)	0.0097 (10)	0.0010 (10)
C1	0.0106 (13)	0.0144 (16)	0.0125 (15)	0.0004 (11)	0.0057 (11)	−0.0015 (11)
C2	0.0111 (13)	0.0083 (15)	0.0136 (14)	−0.0008 (10)	0.0057 (11)	−0.0022 (11)
C3	0.0166 (13)	0.0157 (17)	0.0185 (15)	−0.0007 (12)	0.0112 (12)	−0.0009 (12)
C4	0.0135 (13)	0.0150 (16)	0.0128 (14)	0.0017 (11)	0.0067 (11)	−0.0012 (11)
C5	0.0149 (13)	0.0136 (15)	0.0106 (14)	0.0022 (12)	0.0056 (11)	0.0007 (12)
C6	0.0127 (13)	0.0119 (15)	0.0128 (14)	−0.0023 (11)	0.0075 (11)	0.0004 (11)
C7	0.0161 (13)	0.0162 (17)	0.0165 (15)	0.0017 (12)	0.0068 (12)	−0.0009 (12)
C8	0.0231 (14)	0.0050 (14)	0.0177 (15)	−0.0012 (11)	0.0101 (12)	−0.0002 (11)
C9	0.0166 (13)	0.0175 (17)	0.0171 (15)	−0.0020 (12)	0.0075 (12)	0.0044 (12)
C10	0.0094 (12)	0.0195 (17)	0.0122 (15)	0.0029 (11)	0.0049 (11)	0.0005 (12)

C11	0.0151 (13)	0.0139 (16)	0.0159 (15)	0.0000 (12)	0.0082 (12)	0.0018 (12)
C12	0.0197 (14)	0.0182 (17)	0.0175 (15)	0.0032 (12)	0.0119 (12)	0.0005 (12)
C13	0.0114 (12)	0.0100 (14)	0.0075 (13)	0.0000 (10)	0.0044 (10)	−0.0009 (10)
C14	0.0176 (13)	0.0158 (16)	0.0091 (14)	0.0013 (12)	0.0064 (11)	0.0009 (11)
C15	0.0176 (13)	0.0107 (15)	0.0084 (13)	0.0042 (11)	0.0037 (11)	0.0025 (11)
C16	0.0171 (14)	0.0180 (17)	0.0167 (15)	0.0033 (12)	0.0083 (12)	0.0000 (12)
C17	0.0105 (13)	0.0211 (17)	0.0164 (15)	−0.0028 (12)	0.0051 (11)	0.0027 (13)
C18	0.0173 (14)	0.0139 (16)	0.0154 (15)	−0.0052 (12)	0.0046 (12)	−0.0002 (12)
C19	0.0135 (13)	0.0141 (16)	0.0155 (15)	−0.0006 (12)	0.0057 (11)	−0.0011 (12)
C20	0.0159 (13)	0.0149 (15)	0.0136 (15)	0.0020 (12)	0.0069 (11)	0.0005 (12)

Geometric parameters (Å, º)

O1—C1	1.227 (3)	C7—C8	1.395 (4)
O2—C1	1.307 (3)	C7—H7	0.9500
O2—H2O	0.846 (10)	C8—C9	1.375 (4)
O3—C4	1.249 (3)	C8—H8	0.9500
O4—C11	1.227 (3)	C9—C10	1.401 (4)
O5—C11	1.305 (3)	C9—H9	0.9500
O5—H5O	0.857 (10)	C10—H10	0.9500
O6—C14	1.247 (3)	C11—C12	1.495 (4)
N1—C4	1.350 (3)	C12—C13	1.344 (4)
N1—C5	1.419 (4)	C12—H12	0.9500
N1—H1N	0.879 (10)	C13—C14	1.486 (4)
N2—C14	1.345 (4)	C13—H13	0.9500
N2—C15	1.427 (4)	C15—C20	1.391 (4)
N2—H2N	0.886 (10)	C15—C16	1.394 (4)
C1—C2	1.496 (4)	C16—C17	1.379 (4)
C2—C3	1.335 (4)	C16—H16	0.9500
C2—H2	0.9500	C17—C18	1.394 (4)
C3—C4	1.476 (4)	C17—H17	0.9500
C3—H3	0.9500	C18—C19	1.389 (4)
C5—C10	1.387 (4)	C18—H18	0.9500
C5—C6	1.403 (4)	C19—C20	1.387 (4)
C6—C7	1.377 (4)	C19—H19	0.9500
C6—H6	0.9500	C20—H20	0.9500
C1—O2—H2O	111 (3)	C10—C9—H9	119.7
C11—O5—H5O	112 (2)	C5—C10—C9	119.3 (3)
C4—N1—C5	128.0 (2)	C5—C10—H10	120.3
C4—N1—H1N	114 (2)	C9—C10—H10	120.3
C5—N1—H1N	118 (2)	O4—C11—O5	120.7 (2)
C14—N2—C15	128.4 (2)	O4—C11—C12	118.0 (3)
C14—N2—H2N	117 (2)	O5—C11—C12	121.3 (3)
C15—N2—H2N	115 (2)	C13—C12—C11	132.0 (3)
O1—C1—O2	121.2 (2)	C13—C12—H12	114.0
O1—C1—C2	118.1 (2)	C11—C12—H12	114.0
O2—C1—C2	120.7 (2)	C12—C13—C14	127.9 (2)

C3—C2—C1	132.0 (3)	C12—C13—H13	116.0
C3—C2—H2	114.0	C14—C13—H13	116.0
C1—C2—H2	114.0	O6—C14—N2	123.0 (3)
C2—C3—C4	128.4 (3)	O6—C14—C13	123.6 (3)
C2—C3—H3	115.8	N2—C14—C13	113.4 (2)
C4—C3—H3	115.8	C20—C15—C16	119.9 (3)
O3—C4—N1	122.3 (3)	C20—C15—N2	123.9 (3)
O3—C4—C3	123.1 (3)	C16—C15—N2	116.2 (2)
N1—C4—C3	114.5 (2)	C17—C16—C15	119.7 (3)
C10—C5—C6	119.8 (3)	C17—C16—H16	120.1
C10—C5—N1	123.8 (2)	C15—C16—H16	120.1
C6—C5—N1	116.4 (2)	C16—C17—C18	120.7 (3)
C7—C6—C5	120.3 (3)	C16—C17—H17	119.6
C7—C6—H6	119.8	C18—C17—H17	119.6
C5—C6—H6	119.8	C19—C18—C17	119.4 (3)
C6—C7—C8	119.9 (3)	C19—C18—H18	120.3
C6—C7—H7	120.0	C17—C18—H18	120.3
C8—C7—H7	120.0	C20—C19—C18	120.2 (3)
C9—C8—C7	120.0 (3)	C20—C19—H19	119.9
C9—C8—H8	120.0	C18—C19—H19	119.9
C7—C8—H8	120.0	C19—C20—C15	120.1 (3)
C8—C9—C10	120.6 (3)	C19—C20—H20	120.0
C8—C9—H9	119.7	C15—C20—H20	120.0

O1—C1—C2—C3	174.8 (3)	O4—C11—C12—C13	−175.7 (3)
O2—C1—C2—C3	−5.1 (5)	O5—C11—C12—C13	3.6 (5)
C1—C2—C3—C4	3.8 (5)	C11—C12—C13—C14	−5.2 (5)
C5—N1—C4—O3	2.6 (4)	C15—N2—C14—O6	−1.8 (5)
C5—N1—C4—C3	−176.7 (3)	C15—N2—C14—C13	177.6 (2)
C2—C3—C4—O3	2.7 (5)	C12—C13—C14—O6	−1.1 (5)
C2—C3—C4—N1	−178.0 (3)	C12—C13—C14—N2	179.4 (3)
C4—N1—C5—C10	−9.5 (4)	C14—N2—C15—C20	9.1 (4)
C4—N1—C5—C6	171.4 (3)	C14—N2—C15—C16	−171.5 (3)
C10—C5—C6—C7	2.3 (4)	C20—C15—C16—C17	−0.4 (4)
N1—C5—C6—C7	−178.5 (2)	N2—C15—C16—C17	−179.8 (2)
C5—C6—C7—C8	−0.4 (4)	C15—C16—C17—C18	−0.6 (4)
C6—C7—C8—C9	−1.2 (4)	C16—C17—C18—C19	0.5 (4)
C7—C8—C9—C10	0.9 (4)	C17—C18—C19—C20	0.5 (4)
C6—C5—C10—C9	−2.5 (4)	C18—C19—C20—C15	−1.5 (4)
N1—C5—C10—C9	178.4 (3)	C16—C15—C20—C19	1.5 (4)
C8—C9—C10—C5	0.9 (4)	N2—C15—C20—C19	−179.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2o···O3	0.85 (1)	1.63 (1)	2.475 (3)	172 (4)
O5—H5o···O6	0.86 (1)	1.65 (1)	2.496 (3)	170 (3)

N1—H1n···O4	0.88 (1)	2.00 (1)	2.864 (3)	166 (3)
N2—H2n···O1^{i}	0.89 (1)	1.99 (1)	2.859 (3)	167 (3)

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