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(E)-3-Dimethylamino-1-(4-pyridyl)prop-2-en-1-one

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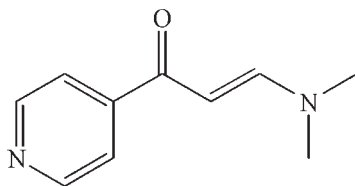
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.040; wR factor = 0.137; data-to-parameter ratio = 14.7.

The title compound, $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}$, is approximately planar, the r.m.s. deviation of the non-H atoms from the mean plane being 0.099 Å.

Related literature

For an isomer of the title compound with the same space group and similar unit-cell parameters, see: Ni *et al.* (2009).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}$

$M_r = 176.22$

Monoclinic, $P2_1/n$

$a = 5.6300$ (11) Å

$b = 22.850$ (5) Å

$c = 7.8400$ (16) Å

$\beta = 107.57$ (3)°

$V = 961.5$ (3) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 0.08$ mm⁻¹

$T = 294$ K

$0.12 \times 0.10 \times 0.08$ mm

Data collection

Bruker APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2004)

$T_{\min} = 0.990$, $T_{\max} = 0.994$

5177 measured reflections

1784 independent reflections

1503 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.137$

$S = 1.00$

1784 reflections

121 parameters

H-atom parameters not refined

$\Delta\rho_{\text{max}} = 0.20$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5024).

References

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supplementary materials

Acta Cryst. (2009). E65, o2104 [doi:10.1107/S1600536809030542]

(*E*)-3-Dimethylamino-1-(4-pyridyl)prop-2-en-1-one

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Comment

As part of our ongoing studies of heteroaromatic compounds (Ni *et al.*, 2009), we now report the synthesis and structure of the title compound, (I).

As shown in Fig. 1, non-hydrogen atoms including the pyridine ring, *N,N*-Dimethylamino, and prop-2-en-1-one are coplanar with the r.m.s deviation of the fitted atoms being 0.099 Å.

Experimental

A mixture of 4-acetylpyridine(10 mmol) and *N,N*-dimethylformamide-dimethyl acetal(40 ml) was refluxed for four hours. After concentration *in vacuo*, recrystallization of the orange residue from ethanol afforded yellow blocks of (I). Anal. Calc. for C₁₀H₁₂N₂O: C 68.10, H 6.81, N 15.89%; Found: C 68.05, H 6.69, N 15.81%.

Refinement

All H atoms were geometrically positioned (C—H = 0.93–0.97Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

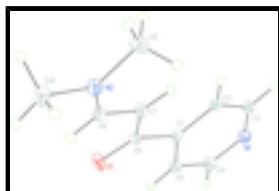


Fig. 1. The molecular structure of (I), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms.

(*E*)-3-Dimethylamino-1-(4-pyridyl)prop-2-en-1-one

Crystal data

C₁₀H₁₂N₂O

$M_r = 176.22$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 5.6300$ (11) Å

$b = 22.850$ (5) Å

$c = 7.8400$ (16) Å

$F_{000} = 376$

$D_x = 1.217$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1784 reflections

$\theta = 1.8$ – 25.5°

$\mu = 0.08$ mm⁻¹

$T = 294$ K

supplementary materials

$\beta = 107.57 (3)^\circ$ Block, yellow
 $V = 961.5 (3) \text{ \AA}^3$ $0.12 \times 0.10 \times 0.08 \text{ mm}$
 $Z = 4$

Data collection

Bruker APEXII CCD diffractometer	1784 independent reflections
Radiation source: fine-focus sealed tube	1503 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.022$
$T = 294 \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -6 \rightarrow 6$
$T_{\text{min}} = 0.990$, $T_{\text{max}} = 0.994$	$k = -27 \rightarrow 26$
5177 measured reflections	$l = -7 \rightarrow 9$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters not refined
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.092P)^2 + 0.1151P]$
$wR(F^2) = 0.137$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} = 0.001$
1784 reflections	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
121 parameters	$\Delta\rho_{\text{min}} = -0.12 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.016 (6)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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C1	0.8254 (2)	0.15312 (5)	0.68372 (16)	0.0403 (3)
C2	0.6652 (3)	0.20055 (6)	0.65592 (17)	0.0451 (4)
H2	0.5490	0.2036	0.7183	0.054*
C3	0.6795 (3)	0.24329 (7)	0.5346 (2)	0.0541 (4)
H3	0.5698	0.2747	0.5180	0.065*
C4	0.9907 (3)	0.19670 (8)	0.4672 (2)	0.0634 (5)
H4	1.1040	0.1947	0.4022	0.076*
C5	0.9919 (3)	0.15168 (7)	0.5851 (2)	0.0533 (4)
H5	1.1034	0.1208	0.5980	0.064*
C6	0.8303 (2)	0.10391 (6)	0.81421 (18)	0.0441 (4)
C7	0.6972 (2)	0.11110 (6)	0.94016 (18)	0.0452 (4)
H7	0.6012	0.1444	0.9377	0.054*
C8	0.7118 (3)	0.06832 (6)	1.06560 (18)	0.0453 (4)
H8	0.8147	0.0367	1.0632	0.054*
C9	0.4227 (3)	0.11224 (8)	1.2011 (2)	0.0668 (5)
H9A	0.5085	0.1490	1.2271	0.100*
H9B	0.3519	0.1028	1.2948	0.100*
H9C	0.2924	0.1150	1.0894	0.100*
C10	0.6374 (3)	0.01980 (7)	1.3199 (2)	0.0641 (5)
H10A	0.7505	-0.0083	1.2966	0.096*
H10B	0.4815	0.0011	1.3112	0.096*
H10C	0.7069	0.0355	1.4380	0.096*
N1	0.8397 (3)	0.24245 (6)	0.44017 (18)	0.0617 (4)
N2	0.5966 (2)	0.06690 (5)	1.18924 (16)	0.0494 (4)
O1	0.9520 (2)	0.05981 (5)	0.80351 (16)	0.0677 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0414 (7)	0.0407 (7)	0.0388 (7)	-0.0052 (5)	0.0120 (5)	-0.0024 (5)
C2	0.0477 (7)	0.0453 (8)	0.0433 (7)	-0.0010 (6)	0.0153 (6)	-0.0018 (6)
C3	0.0581 (9)	0.0476 (8)	0.0541 (9)	0.0035 (6)	0.0131 (7)	0.0068 (6)
C4	0.0583 (9)	0.0715 (11)	0.0699 (10)	0.0001 (8)	0.0337 (8)	0.0178 (8)
C5	0.0500 (8)	0.0541 (9)	0.0623 (9)	0.0035 (6)	0.0268 (7)	0.0092 (7)
C6	0.0480 (7)	0.0410 (7)	0.0460 (7)	0.0005 (5)	0.0184 (6)	0.0004 (6)
C7	0.0498 (7)	0.0429 (7)	0.0467 (7)	0.0020 (6)	0.0202 (6)	0.0009 (5)
C8	0.0499 (8)	0.0442 (8)	0.0460 (8)	-0.0016 (6)	0.0210 (6)	-0.0037 (6)
C9	0.0651 (10)	0.0810 (12)	0.0631 (10)	0.0146 (8)	0.0326 (8)	0.0008 (8)
C10	0.0914 (12)	0.0553 (9)	0.0583 (9)	-0.0050 (8)	0.0415 (9)	0.0036 (7)
N1	0.0633 (8)	0.0598 (8)	0.0646 (8)	-0.0018 (6)	0.0232 (7)	0.0176 (6)
N2	0.0576 (7)	0.0507 (7)	0.0476 (7)	0.0002 (5)	0.0274 (6)	0.0012 (5)
O1	0.0928 (9)	0.0519 (7)	0.0772 (8)	0.0237 (6)	0.0538 (7)	0.0171 (5)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.3846 (18)	C7—C8	1.3713 (19)
C1—C5	1.3842 (19)	C7—H7	0.9300
C1—C6	1.5148 (18)	C8—N2	1.3193 (17)
C2—C3	1.382 (2)	C8—H8	0.9300

supplementary materials

C2—H2	0.9300	C9—N2	1.4476 (19)
C3—N1	1.329 (2)	C9—H9A	0.9600
C3—H3	0.9300	C9—H9B	0.9600
C4—N1	1.323 (2)	C9—H9C	0.9600
C4—C5	1.382 (2)	C10—N2	1.4555 (19)
C4—H4	0.9300	C10—H10A	0.9600
C5—H5	0.9300	C10—H10B	0.9600
C6—O1	1.2357 (16)	C10—H10C	0.9600
C6—C7	1.4180 (18)		
C2—C1—C5	116.72 (12)	C6—C7—H7	120.4
C2—C1—C6	124.44 (12)	N2—C8—C7	127.45 (13)
C5—C1—C6	118.84 (12)	N2—C8—H8	116.3
C1—C2—C3	119.39 (13)	C7—C8—H8	116.3
C1—C2—H2	120.3	N2—C9—H9A	109.5
C3—C2—H2	120.3	N2—C9—H9B	109.5
N1—C3—C2	124.31 (14)	H9A—C9—H9B	109.5
N1—C3—H3	117.8	N2—C9—H9C	109.5
C2—C3—H3	117.8	H9A—C9—H9C	109.5
N1—C4—C5	124.67 (14)	H9B—C9—H9C	109.5
N1—C4—H4	117.7	N2—C10—H10A	109.5
C5—C4—H4	117.7	N2—C10—H10B	109.5
C4—C5—C1	119.24 (14)	H10A—C10—H10B	109.5
C4—C5—H5	120.4	N2—C10—H10C	109.5
C1—C5—H5	120.4	H10A—C10—H10C	109.5
O1—C6—C7	124.21 (12)	H10B—C10—H10C	109.5
O1—C6—C1	117.19 (12)	C4—N1—C3	115.67 (13)
C7—C6—C1	118.60 (11)	C8—N2—C9	121.45 (12)
C8—C7—C6	119.15 (12)	C8—N2—C10	121.81 (13)
C8—C7—H7	120.4	C9—N2—C10	116.74 (12)

Fig. 1

