Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Chloro-1-[(4-nitrophenyl)hydrazinylidene]propan-2-one

Abdullah M. Asiri,[a,b] Abdulrahman O. Al-Youbi,[a] Mohie E. M. Zayed[a] and Seik Weng Ng[c,a]*

[a]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia, [b]The Center of Excellence for Advanced Materials Research, King Abdul Aziz University, PO Box 8020 Jeddah, Saudi Arabia, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

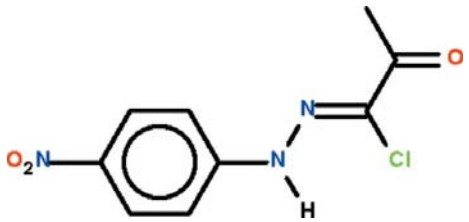
Received 29 June 2011; accepted 3 July 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.152; data-to-parameter ratio = 14.0.

The non-H atoms of the title compound, $C_9H_8ClN_3O_3$, lie approximately on a plane (r.m.s. deviation = 0.111 Å), and the C=N double bond has a Z configuration. In the crystal, adjacent molecules are linked by an N—H···$O_{carbonyl}$ hydrogen bond, forming a chain running along [101].

Related literature

For the synthesis, see: Benincori *et al.* (1990); Sayed *et al.* (2002). For background to the title compound, see: Asiri *et al.* (2010).



Experimental

Crystal data

$C_9H_8ClN_3O_3$
M_r = 241.63
Monoclinic, $P2_1/n$
a = 7.0628 (3) Å
b = 13.4182 (5) Å
c = 11.2884 (5) Å
β = 95.589 (4)°
V = 1064.72 (8) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.19 mm^{-1}
T = 100 K
0.20 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.568, T_{max} = 0.857
4113 measured reflections
2105 independent reflections
1839 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 1.09
2105 reflections
150 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.85 (4)	2.26 (4)	3.000 (3)	145 (3)

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5261).

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