Marole M Maluleka* and Malose J Mphahlele*

Crystal structure of (*E*)-1-(2-nitrophenyl)-3-phenylprop-2-en-1-one, C₁₅H₁₁NO₃

Table 1: Data collection and handling.

Crystal:	Yellow needle
Size:	0.36 × 0.16 × 0.12 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.10 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Venture Photon, ω
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	46,990, 2281, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2091
$N(\text{param})_{\text{refined}}$:	172
Programs:	Bruker [1], WinGX/ORTEP [2], SHELX [3]

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Abstract

C₁₅H₁₁NO₃, $P2_1/c$ (no. 14), $a = 5.4092(2)$ Å, $b = 23.9605(8)$ Å, $c = 9.4887(3)$ Å, $\beta = 96.080(1)^\circ$, $V = 1222.89(7)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0358$, $wR_{\text{ref}}(F^2) = 0.0888$, $T = 173(2)$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of 2-nitroacetophenone (2.0 g, 12.1 mmol) and benzaldehyde derivative (1.54 g, 14.5 mmol) in the presence of 5% KOH (5 mL) in ethanol (20 mL) was stirred at room

temperature (RT) for 78 h. The mixture was acidified dropwise with concentrated hydrochloric acid and the resultant precipitate was filtered off and washed with cold water. Crystals of the title compound were obtained by recrystallization in ethanol.

Experimental details

X-ray single crystal data was collected on a Bruker D8 Venture diffractometer at 173 K using an Oxford Cryostream 600 low-temperature controller. Data reduction was carried out using the program SAINT+, version 6.02 [1] and empirical absorption corrections were made using SADABS [1]. The structure was solved in the WinGX [2] Suite of programs, using intrinsic phasing through SHELXT [3] and refined using full-matrix least-squares/difference Fourier techniques on F^2 using SHELXL-2017 [3]. All carbon-bound hydrogen atoms were placed at idealized positions and refined as riding atoms with isotropic parameters 1.2 times those of their parent atoms.

Comment

Chalcones (1,3-diphenylprop-2-ene-1-ones) are the precursors of flavonoids and isoflavonoids, which are abundant in edible plants [4]. They display a wide range of pharmacological properties, and some derivatives have found application in the treatment of several human disorders

*Corresponding authors: Marole M Maluleka, Department of Chemistry, Faculty of Science and Agriculture, School of Physical and Mineral Science, University of Limpopo, Private bag X1106, Polokwane, Sovenga, 0727, South Africa, E-mail: marole.maluleka@ul.ac.za. <https://orcid.org/0000-0002-3301-8421> (M.M. Maluleka); and Malose J Mphahlele, Department of Chemistry, College of Science Engineering and Technology, University of South Africa, Private Bag X06, Johannesburg, Florida Park, 1710, South Africa, E-mail: mphahmj@unisa.ac.za. <https://orcid.org/0000-0002-6018-5671> (M.J. Mphahlele)

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.2115 (2)	0.65511 (5)	0.17385 (13)	0.0265 (3)
C2	0.1734 (2)	0.71158 (5)	0.19862 (13)	0.0268 (3)
C3	0.3018 (3)	0.75327 (6)	0.13585 (15)	0.0346 (3)
H3	0.272488	0.791456	0.155255	0.042*
C4	0.4731 (3)	0.73827 (7)	0.04465 (16)	0.0402 (4)
H4	0.564084	0.766231	0.001381	0.048*
C5	0.5121 (3)	0.68263 (7)	0.01636 (15)	0.0409 (4)
H5	0.628736	0.672464	−0.047268	0.049*
C6	0.3829 (3)	0.64170 (6)	0.07984 (14)	0.0347 (3)
H6	0.41161	0.603614	0.058951	0.042*
C7	0.0812 (2)	0.60745 (5)	0.23931 (14)	0.0295 (3)
C8	0.1829 (2)	0.58635 (5)	0.37817 (14)	0.0307 (3)
H8	0.089866	0.558842	0.42172	0.037*
C9	0.3969 (2)	0.60304 (5)	0.44772 (13)	0.0274 (3)
H9	0.48529	0.631365	0.404089	0.033*
C10	0.5096 (2)	0.58215 (5)	0.58452 (13)	0.0273 (3)
C11	0.7317 (3)	0.60567 (6)	0.64539 (15)	0.0340 (3)
H11	0.807931	0.634699	0.597251	0.041*
C12	0.8420 (3)	0.58710 (6)	0.77533 (16)	0.0407 (4)
H12	0.993013	0.603489	0.815803	0.049*
C13	0.7334 (3)	0.54486 (6)	0.84627 (15)	0.0408 (4)
H13	0.80954	0.53212	0.935272	0.049*
C14	0.5138 (3)	0.52125 (6)	0.78737 (16)	0.0413 (4)
H14	0.438899	0.492215	0.836159	0.05*
C15	0.4023 (3)	0.53951 (6)	0.65810 (15)	0.0354 (3)
H15	0.251061	0.522933	0.618674	0.043*
N1	−0.0103 (2)	0.72862 (5)	0.29322 (12)	0.0307 (3)
O1	−0.0475 (2)	0.77829 (4)	0.30923 (13)	0.0504 (3)
O2	−0.11979 (19)	0.69190 (4)	0.35205 (11)	0.0408 (3)
O3	−0.09393 (19)	0.58472 (4)	0.17099 (12)	0.0439 (3)

including cancer, diabetes, cardiovascular and neurological diseases as well as other chronic diseases [4]. Their bioactivity is correlated with the different electron-donor and electron-acceptor groups attached to the aromatic rings on either side of the α,β-unsaturated carbonyl (−CO−CH=CH−) framework [5]. Although the presence of the carbon–carbon double bond may give rise to *trans*- and *cis*-isomeric forms, the *trans* geometry is the thermodynamically more stable and favourable geometry [6]. Their conjugated ketoethylenic scaffold is involved in many biochemical signalling pathways in cell as a Michael acceptor [7]. The conjugated keto-ethylenic scaffold and a completely delocalized π-electron system have also been found to reduce their redox potentials and make chalcones to be prone to electron transfer reactions [8]. Chalcones are not only of interest from the medicinal chemistry context, their conformations and crystalline structures attract attention to explore non-covalent (intramolecular and intermolecular) interactions,

control molecular conformations, and improve their physicochemical and optical properties. A number of synthetic routes have been reported for synthesis of chalcones [5]. The Claisen–Schmidt condensation of acetophenone and benzaldehyde derivatives under aqueous basic or acidic conditions remains the most popular and sure-fire method for their synthesis. This methodology has been adapted for the synthesis of (*E*)-1-(2-nitrophenyl)-3-phenylprop-2-en-1-one. Its crystal structure is reported in this work to be added to the dataset of molecules based on the nitro substituted chalcones.

The crystal structure shows the phenyl ring and the 2-nitroacetophenone fragment oriented in the *trans* geometry around the ethylenic framework. The 2-nitrophenyl group (A-ring) deviates from coplanarity of the conjugated system with torsion angle, C(6)–C(1)–C(7)–C(8), of 94.54(15) Å to minimize electrostatic repulsions between oxygen atoms of the nitro and the carbonyl groups. Bond lengths are all in the expected ranges [9]. The molecule is stabilized by intermolecular π-stacking and C–H⋯O interactions.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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