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The crystal structure of (*E*)-3-(furan-2-yl)acrylonitrile, C₇H₅NO

<https://doi.org/10.1515/ncrs-2022-0036>

Received January 20, 2022; accepted February 21, 2022;
published online March 7, 2022

Abstract

C₇H₅NO, monoclinic, *P*₂₁/*n* (no. 14), *a* = 3.7589(5) Å, *b* = 19.493(2) Å, *c* = 8.4180(10) Å, *V* = 601.98(13) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0502, *wR*_{ref}(*F*²) = 0.1274, *T* = 170 K.

CCDC no.: 2069214

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

Source of material

The substrate 2-furanacrylamide (1.0 mmol), (EtO)₃SiH (3.0 mmol), phenylselenophenol iron complex (2 mol%) as catalyst and tetrahydrofuran (THF) (2 mL) were added into a 25 mL Schlenk tube in a nitrogen atmosphere at room temperature. The reaction mixture was stirred at 60 °C for 24 h. The reaction progress was detected by gas chromatography (GC) and thin layer chromatography (TLC). After the reaction, the product was extracted using petroleum ether (10 mL) three times, and the organic phase were combined together and dried with anhydrous Na₂SO₄. The organic solvents were removed by vacuum distillation.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.12 × 0.08 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.09 mm ⁻¹
Diffractometer, scan mode:	BRUKER APEX-II, φ and ω
θ _{max} , completeness:	26.5°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	6761, 1253, 0.075
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2σ(<i>I</i> _{obs}), 945
<i>N</i> (param) _{refined} :	82
Programs:	BRUKER [1], OLEX2 [2], SHELX [3,4]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.3952 (5)	0.68836 (10)	0.7127 (2)	0.0279 (5)
H1	0.380367	0.709650	0.812593	0.033*
C2	0.4694 (5)	0.72158 (10)	0.5732 (2)	0.0290 (5)
H2	0.513857	0.769072	0.561137	0.035*
C3	0.4638 (6)	0.67189 (10)	0.4615 (2)	0.0299 (5)
H3	0.504792	0.679362	0.355424	0.036*
C4	0.3496 (5)	0.62080 (10)	0.6770 (2)	0.0242 (5)
C5	0.2630 (5)	0.56344 (10)	0.7672 (2)	0.0249 (5)
H5	0.217764	0.572413	0.871981	0.030*
C6	0.2400 (5)	0.49831 (10)	0.7170 (2)	0.0267 (5)
H6	0.288485	0.487902	0.613531	0.032*
C7	0.1454 (5)	0.44370 (10)	0.8131 (2)	0.0266 (5)
N1	0.0695 (5)	0.39881 (9)	0.8877 (2)	0.0326 (5)
O1	0.3916 (4)	0.60939 (7)	0.52050 (15)	0.0281 (4)

Crude products were purified by gel column chromatography and finally recrystallized to obtain the title compound.

Experimental details

All hydrogen atoms were placed in calculated positions and refined as riding atoms. The *U*_{iso} values were constrained to be 1.2*U*_{eq}. All the H atoms were refined as riding on their parent atom.

Comment

Furan derivatives have a unique status and important feature in a variety of natural products [5, 6]. They are widely

used in some important commercial products, like dyes, essential oils, cosmetic, industrial preservative, bio-regulators, photosensitizers, fire retardants, and flavoring compounds [7–10]. Additionally, furan analogues show abundant pharmacological properties, like anti-depressant, anti-inflammatory, anti-hypertensive, anti-ageing, anti-cancer, anti-ulcer, anti-oxidation, and anti-glaucoma effects [11–16], which engage the attention of medicinal chemists to synthesize a series of furan-based derivatives [5]. For example, furan-2-carboxamide and 2-furyl acetonitrile derivatives [6, 17] have found use as key intermediates to synthesize new candidates for anti-cancer drugs.

The asymmetric unit of the title structure contains one molecule (see the Figure). Weak intermolecular C–H···O and C–H···N hydrogen bonds are observed. Additionally, a weak intramolecular hydrogen C6–H6···O1 bond interaction is also formed between O1 and H6 atoms. The C7–N1 distance is 1.149(3) Å, which indicates a C–N triple bond. The three N1–C7–C6 atoms with the bond angle of 178.5(3)° are almost in a straight line. Weak hydrogen bond interactions connect the molecular structures into a three-dimensional network. For example, there is a weak C–H···O interaction (2.6282(15) Å) between H6 atom and the O1 atom of the adjacent molecule. The similar intermolecular interaction (C–H···N, 2.5958(18) Å) was observed in the H2 and N1 atoms. All geometric parameters are as expected [18].

Acknowledgements: We gratefully acknowledge support by the key scientific research projects of colleges and universities in Henan Province for financial support (22A430032).

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: Key Scientific Research Projects of Colleges and Universities in Henan Province for financial support (22A430032).

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

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