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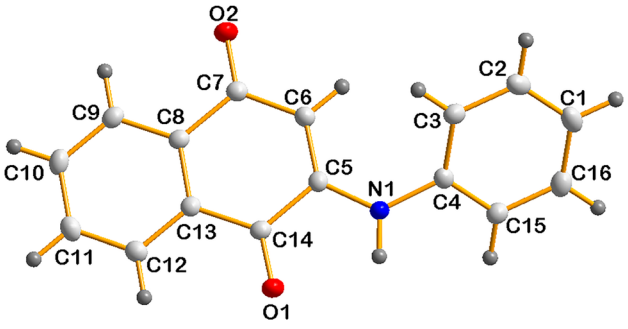
The crystal structure of 2-anilino-1,4-naphthoquinone, $C_{10}H_{11}NO_2$



https://doi.org/10.1515/ncrs-2023-0338
Received July 19, 2023; accepted August 17, 2023;
published online September 4, 2023

Abstract

$C_{10}H_{11}NO_2$, monoclinic, $P2_1/n$ (no. 14), a = 3.7617(3) Å, b = 12.9267(10) Å, c = 23.4609(17) Å, β = 92.337(3)°, V = 1139.87(15) Å^3, Z = 4, $R_{gt}(F)$ = 0.0413, $wR_{ref}(F^2)$ = 0.1071, T = 100 K.

CCDC no.: 2289189

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.

1 Source of materials

The 2-anilino-1,4-naphthoquinone was purchased from Sigma Aldrich and then dissolved in 3 mL acetone. The solution was kept to room temperature for crystallization. Red cuboid crystals were obtained.

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Table 1: Data collection and handling.

Crystal:	Red needle
Size:	0.43 × 0.08 × 0.04 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.10 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture 5K Kappa Photon III
θ_{max}, completeness:	28.3°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	19,336, 2811, 0.049
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2294
$N(param)_{refined}$:	176
Programs:	SHELX [1], Bruker [2], Olex2 [3], Diamond [4]

2 Experimental details

The aromatic H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with fixed C–H distances for aromatic C–H of 0.93 Å (C–H) [$U_{iso}(H) = 1.2U_{eq}$]. The N1–H1 hydrogen was placed according to the Fourier electron difference density map. The graphics were obtained using the DIAMOND [4] program with 50 % probability ellipsoids. The highest peak is located 0.68 Å from C6 and the deepest hole is situated 0.61 Å from C14 respectively.

3 Comment

It is known that cancer is one of the diseases that have a great impact on our daily lives, and much scientific research is being conducted in order to limit and get rid of this incurable disease.

Epidermal growth factor receptor (EGFR) has been recognized as a very important aim for anticancer drug development. The 2-anilino-1,4-naphthoquinone and its derivatives have been shown to be related to be potential for their anticancer and EGFR inhibitor [5]. One of the most important naphthalene derivatives is naphthoquinone, with two carbonyl groups it is a privileged scaffold found in many classes of naturally occurring bioactive compounds and it has been used and its derivatives for cancer treatment [6, 7]. Different molecular mechanisms with regard to anticancer activities of the naphthoquinone-based compounds have been described [8–10]. In our laboratory, we have many results on the possibility of coordinating such compounds with the platinum group metals to increase the possibility to have an impact on cancer [11, 12].

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0055 (3)	0.58217 (7)	0.54884 (4)	0.0222 (2)
O2	0.7062 (3)	0.53632 (7)	0.75009 (4)	0.0244 (2)
N1	0.2742 (3)	0.39814 (8)	0.57225 (5)	0.0181 (2)
C1	0.5409 (4)	0.08329 (10)	0.58117 (6)	0.0246 (3)
H1A	0.601030	0.011946	0.582759	0.029*
C2	0.4078 (4)	0.13178 (10)	0.62849 (6)	0.0238 (3)
H2	0.376798	0.093575	0.662524	0.029*
C3	0.3196 (4)	0.23610 (10)	0.62628 (5)	0.0202 (3)
H3	0.225596	0.269034	0.658583	0.024*
C4	0.3695 (3)	0.29224 (10)	0.57662 (5)	0.0176 (3)
C5	0.3273 (3)	0.47199 (9)	0.61246 (5)	0.0165 (2)
C6	0.5037 (3)	0.46219 (9)	0.66401 (5)	0.0181 (3)
H6	0.601033	0.396728	0.674412	0.022*
C7	0.5485 (3)	0.54705 (9)	0.70343 (5)	0.0174 (3)
C8	0.4056 (3)	0.65055 (9)	0.68593 (5)	0.0161 (2)
C9	0.4586 (3)	0.73502 (10)	0.72194 (5)	0.0188 (3)
H9	0.579777	0.726369	0.757950	0.023*
C10	0.3345 (3)	0.83196 (10)	0.70533 (6)	0.0211 (3)
H10	0.370949	0.889558	0.730028	0.025*
C11	0.1571 (3)	0.84512 (10)	0.65265 (6)	0.0211 (3)
H11	0.071867	0.911634	0.641588	0.025*
C12	0.1041 (3)	0.76178 (10)	0.61629 (6)	0.0188 (3)
H12	−0.016143	0.770941	0.580245	0.023*
C13	0.2288 (3)	0.66391 (9)	0.63293 (5)	0.0163 (2)
C14	0.1717 (3)	0.57481 (9)	0.59454 (5)	0.0165 (3)
C15	0.5014 (3)	0.24358 (10)	0.52911 (5)	0.0195 (3)
H15	0.533653	0.281620	0.495064	0.023*
C16	0.5859 (4)	0.13895 (10)	0.53164 (6)	0.0235 (3)
H16	0.675241	0.105472	0.499134	0.028*
H1	0.182 (5)	0.4211 (14)	0.5380 (8)	0.032 (5)*

There is one molecule in the asymmetric unit of the title structure. In the title structure, the O1–C14, O2–C7, N1–C4 and N1–C5 bond lengths were determined as 1.2219(17), 1.2312(17), 1.4176(17) and 1.3504(17) respectively. The C5–N1–C4, C3–C4–N1, C15–C4–N1, N1–C5–C6, N1–C5–C14, O2–C7–C6, O2–C7–C8, O1–C14–C5 and O1–C14–C13 bond angles were determined as 127.04(12), 121.45(12), 118.47(12), 127.41(12), 112.59(12), 121.66(12), 120.04(12) and 119.53(12) respectively. All parameters are in the expected ranges [13–15].

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

Research funding: The authors acknowledge funding under the Swiss-South Africa joint research program (SSAJRP) from the SANRF (A. Roodt: UID: 107802) as well as from the Competitive Program for Rated Researchers of the SANRF (A. Roodt: UID: 111698), from the South African Department of Science Innovation (DSI) and the Department of Science and Technology (DST) respectively, "Department of Science and Innovation, Republic of South Africa" and "Department of Science and Technology, Republic of South Africa".

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

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