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Synthesis and crystal structure of (1*E*,2*E*)-3-(anthracen-9-yl)-1-(4-methoxyphenyl)prop-2-en-1-one oxime, C₂₄H₁₉NO₂

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Abstract

C₂₄H₁₉NO₂, triclinic, $P\bar{1}$ (no. 2), $a = 8.3580(17)$ Å, $b = 10.220(2)$ Å, $c = 11.227(2)$ Å, $\alpha = 85.25(3)^\circ$, $\beta = 81.35(3)^\circ$, $\gamma = 88.72(3)^\circ$, $V = 944.8(3)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0873$, $wR_{ref}(F^2) = 0.1988$, $T = 293$ K.

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Table 1: Data collection and handling.

Crystal:	Yellow needle
Size:	0.20 × 0.10 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Enraf Nonius TurboCAD4, ω
θ_{max} , completeness:	25.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	3475, 3475, 0.030
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1442
$N(param)_{refined}$:	244
Programs:	CAD-4 [1, 2], SHELX [3], DIAMOND [4]

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 materials

The title compound (1*E*,2*E*)-3-(anthracen-9-yl)-1-(4-methoxyphenyl)prop-2-en-1-one oxime (AMPO) was obtained by a reported synthetic protocol in two steps with a 60% yield [5]. Single crystals of light yellow color were grown from acetone at room temperature via slow evaporation.

Experimental details

The hydrogen atoms bonded to the carbon atoms were placed in calculated positions and refined as riding mode, with C–H = 0.96 Å with $U_{iso}(H) = 1.2 U_{eq}(C)$. For the OH and the CH₃ group the SHELX commands AFIX 83 and AFIX 33 were used respectively [3].

Comment

Oximes are organic compounds, which found diverse applications in a variety of products due to the ease of

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

Atom	x	y	z	U _{iso} */U _{eq}
N	0.9228 (5)	0.1215 (4)	0.5387 (3)	0.0541 (10)
O1	0.9446 (5)	0.3178 (3)	1.0508 (3)	0.0823 (12)
C1	0.5180 (6)	0.3386 (5)	0.6782 (5)	0.0622 (14)
O2	0.9030 (4)	0.1052 (3)	0.4187 (3)	0.0741 (11)
H2A	0.9310	0.0306	0.4022	0.111*
C2	0.5042 (7)	0.2203 (5)	0.6215 (5)	0.0736 (16)
H2B	0.5596	0.2111	0.5443	0.088*
C3	0.4111 (8)	0.1218 (6)	0.6793 (7)	0.094 (2)
H3A	0.4036	0.0455	0.6408	0.113*
C4	0.3241 (8)	0.1306 (8)	0.7971 (8)	0.120 (3)
H4A	0.2633	0.0604	0.8365	0.144*
C5	0.3316 (8)	0.2434 (7)	0.8509 (7)	0.108 (2)
H5A	0.2744	0.2502	0.9279	0.129*
C6	0.4229 (6)	0.3501 (6)	0.7942 (5)	0.0726 (16)
C7	0.4188 (6)	0.4674 (6)	0.8495 (5)	0.0779 (17)
H7A	0.3538	0.4747	0.9236	0.093*
C8	0.5116 (6)	0.5746 (6)	0.7947 (5)	0.0687 (15)
C9	0.5047 (8)	0.6968 (7)	0.8506 (6)	0.0907 (19)
H9A	0.4402	0.7040	0.9249	0.109*
C10	0.5897 (8)	0.7993 (7)	0.7970 (7)	0.100 (2)
H10A	0.5852	0.8772	0.8349	0.120*
C11	0.6861 (8)	0.7916 (6)	0.6841 (6)	0.0895 (19)
H11A	0.7444	0.8643	0.6474	0.107*
C12	0.6943 (6)	0.6780 (4)	0.6284 (5)	0.0659 (14)
H12A	0.7603	0.6742	0.5542	0.079*
C13	0.6066 (5)	0.5659 (5)	0.6790 (4)	0.0534 (12)
C14	0.6145 (6)	0.4465 (5)	0.6263 (4)	0.0566 (13)
C15	0.7210 (6)	0.4350 (4)	0.5099 (4)	0.0585 (13)
H15A	0.7077	0.4980	0.4473	0.070*
C16	0.8346 (5)	0.3427 (4)	0.4858 (4)	0.0505 (12)
H16A	0.8893	0.3455	0.4071	0.061*
C17	0.8811 (5)	0.2380 (4)	0.5707 (4)	0.0451 (10)
C18	0.8905 (5)	0.2586 (4)	0.7002 (3)	0.0411 (10)
C19	0.9382 (6)	0.3776 (4)	0.7314 (4)	0.0536 (12)
H19A	0.9591	0.4474	0.6729	0.064*
C20	0.9551 (6)	0.3933 (5)	0.8512 (4)	0.0630 (14)
H20A	0.9891	0.4730	0.8725	0.076*
C21	0.9212 (6)	0.2899 (5)	0.9377 (4)	0.0575 (13)
C22	0.8674 (6)	0.1731 (4)	0.9089 (4)	0.0539 (12)
H22A	0.8400	0.1056	0.9688	0.065*
C23	0.8539 (6)	0.1561 (4)	0.7901 (4)	0.0548 (12)
H23A	0.8203	0.0759	0.7697	0.066*
C24	0.9312 (8)	0.2135 (5)	1.1430 (4)	0.091 (2)
H24A	0.9502	0.2460	1.2174	0.137*
H24B	0.8246	0.1773	1.1533	0.137*
H24C	1.0098	0.1465	1.1207	0.137*

attaching functional groups [6]. Oximes found extensive applications in metallo-assemblies and sensors [7, 8], decoration of nanoparticles [9] as biological scaffold [10] and in the preparation of protein conjugates [11].

In the structure, the neighboring AMPO molecules associate through non-classical C24–H24...O2 hydrogen bonds forming a chain along the *b* axis. Furthermore, the two chains are associated through O2–H2...N hydrogen bonds forming a 2D structure. The anthracene rings form a slipped arrangement with a centroid–centroid distance of 5.365 Å indicating no π – π interaction between neighboring rings.

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