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The crystal structure of 4-((2-(4,5-dihydro-1,5-diphenyl-1*H*-pyrazol-3-yl)anthracen-10-yl)methyl)morpholine, C₃₄H₃₁N₃O

<https://doi.org/10.1515/ncrs-2018-0463>

Received October 30, 2018; accepted December 17, 2018; available online February 4, 2019

Abstract

C₃₄H₃₁N₃O, monoclinic, *P*₂₁/*c* (no. 14), *a* = 26.803(5) Å, *b* = 5.8243(12) Å, *c* = 16.893(3) Å, β = 98.53(3)°, *V* = 2608.1(9) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0759, *wR*_{ref}(*F*²) = 0.2028, *T* = 113(2) K.

CCDC no.: 1885555

Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized by the reaction of 1-(10-(morpholinomethyl)anthracen-2-yl)-3-phenylprop-2-en-1-one (0.5 g, 1.2 mmol), phenylhydrazine (0.199 g, 1.18 mmol) and a grain of NaOH in methanol [4]. The mixture refluxed for 16 hours. After cooling water was added and filtered, washed with water and purified methanol to get a yellow

Table 1: Data collection and handling.

Crystal:	Yellow rod
Size:	0.20 × 0.18 × 0.10 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.08 mm ^{−1}
Diffractometer, scan mode:	Bruker APEX-II CCD,
θ _{max} , completeness:	27.1°, 99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	19073, 5694, 0.065
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 3784
<i>N</i> (<i>param</i>) _{refined} :	344
Programs:	Bruker [1], SHELX [2, 3]

solid (0.21 g, 35%). ¹H NMR (400 MHz, CDCl₃, 25 °C): δ 2.624 (t, *J* = 4.8 Hz, *J* = 4.4 Hz, 4H), 3.287–3.346 (m, 1H), 3.653 (t, *J* = 4.4 Hz, *J* = 4.8 Hz, 4H), 3.963–3.036 (m, 1H), 4.437(s, 2H), 5.347–5.395 (m, 1H), 6.802–6.843 (m, 1H), 7.148 (t, *J* = 8.5 Hz, 2H), 7.204–7.244 (m, 2H), 7.267–7.303 (m, 2H), 7.364 (t, *J* = 4.08 Hz, 3H), 7.457–7.494 (m, 1H), 7.512–7.514 (m, 1H), 7.840 (d, *J* = 2 Hz, 1H), 7.975 (d, *J* = 8.17 Hz, 1H), 8.258–8.286 (m, 1H), 8.339 (s, 1H), 8.455–8.49 (m, 2H). ¹³C NMR (100 MHz, CDCl₃): δ 43.125, 53.564, 54.44, 64.468, 67.059, 76.626, 76.943, 77.261, 113.387, 119.197, 123.363, 125.017, 125.199, 125.714, 125.783, 127.541, 127.665, 128.817, 128.88, 129.104, 129.361, 130.972, 131.099, 131.645, 131.736, 142.439, 144.484, 146.466.

Experimental details

The structure was solved by Direct Methods, and the non-hydrogen atoms were subjected to anisotropic refinement [2].

Comment

Supramolecular chemistry plays an important role in molecular electronics [5] and biological system probes [6, 7]. Anthracene, as an important fluorescent group, has been widely used in supramolecular chemistry [8–10]. In the title structure the dihedral angles between the two benzenes and pyrazoline are 89.38(18)° and 2.15(17)°. The anthracene moiety is almost on the same plane with pyrazoline ring, and the dihedral angle is 8.4(1)°. The crystal structure features π–π interactions involving the phenyl and anthracene group. In the crystal, π–π and van der Waals interactions are effective in molecular packing.

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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}
O1	1.02187(6)	0.4141(3)	0.13233(10)	0.0427(5)
N1	0.67041(7)	−0.1348(3)	0.30233(11)	0.0350(5)
N2	0.70311(7)	−0.0084(3)	0.26237(11)	0.0349(5)
N3	0.91564(7)	0.3937(3)	0.07350(10)	0.0305(4)
C1	0.65384(9)	−0.0466(4)	0.37057(13)	0.0319(5)
C2	0.61778(9)	−0.1673(4)	0.40655(13)	0.0370(6)
H2	0.6043	−0.3069	0.3835	0.044*
C3	0.60178(10)	−0.0844(4)	0.47528(14)	0.0423(6)
H3	0.5774	−0.1677	0.4992	0.051*
C4	0.62108(10)	0.1197(5)	0.50942(14)	0.0457(7)
H4	0.6097	0.1776	0.5562	0.055*
C5	0.65702(10)	0.2381(4)	0.47491(14)	0.0456(7)
H5	0.6703	0.3775	0.4985	0.055*
C6	0.67418(9)	0.1567(4)	0.40608(13)	0.0382(6)
H6	0.6994	0.2383	0.3836	0.046*
C7	0.64806(9)	−0.3305(4)	0.25459(13)	0.0347(5)
H7	0.6488	−0.4708	0.2889	0.042*
C8	0.59453(9)	−0.2842(4)	0.21367(13)	0.0328(5)
C9	0.58220(9)	−0.0798(4)	0.17244(14)	0.0400(6)
H9	0.6068	0.0381	0.1735	0.048*
C10	0.53434(10)	−0.0470(4)	0.12980(15)	0.0447(6)
H10	0.5265	0.0927	0.1016	0.054*
C11	0.49793(10)	−0.2165(5)	0.12808(16)	0.0509(7)
H11	0.4653	−0.1949	0.0982	0.061*
C12	0.50956(10)	−0.4171(5)	0.17026(17)	0.0526(7)
H12	0.4845	−0.5324	0.1708	0.063*
C13	0.55760(10)	−0.4510(4)	0.21185(15)	0.0439(6)
H13	0.5653	−0.5914	0.2396	0.053*
C14	0.68558(9)	−0.3566(4)	0.19448(14)	0.0376(6)
H14A	0.7098	−0.4825	0.2102	0.045*
H14B	0.6679	−0.3854	0.1397	0.045*
C15	0.71148(8)	−0.1263(4)	0.20025(13)	0.0320(5)
C16	0.74461(8)	−0.0408(4)	0.14579(13)	0.0326(5)
C17	0.77491(8)	0.1598(4)	0.16592(13)	0.0337(5)
H17	0.7736	0.2350	0.2155	0.040*
C18	0.80550(9)	0.2441(4)	0.11521(13)	0.0347(5)
H18	0.8250	0.3773	0.1304	0.042*
C19	0.80914(8)	0.1383(4)	0.03960(13)	0.0321(5)
C20	0.84087(8)	0.2246(4)	−0.01306(13)	0.0318(5)
C21	0.84375(8)	0.1085(4)	−0.08627(13)	0.0324(5)
C22	0.87541(9)	0.1822(4)	−0.14275(13)	0.0378(6)
H22	0.8945	0.3193	−0.1329	0.045*
C23	0.87855(9)	0.0589(5)	−0.21042(14)	0.0434(6)
H23	0.8995	0.1124	−0.2472	0.052*
C24	0.85100(9)	−0.1483(5)	−0.22675(13)	0.0417(6)
H24	0.8545	−0.2351	−0.2732	0.050*
C25	0.81980(9)	−0.2221(4)	−0.17633(13)	0.0390(6)
H25	0.8012	−0.3598	−0.1881	0.047*
C26	0.81427(8)	−0.0963(4)	−0.10545(12)	0.0317(5)
C27	0.78196(8)	−0.1739(4)	−0.05308(13)	0.0342(5)
H27	0.7615	−0.3049	−0.0673	0.041*
C28	0.77905(8)	−0.0637(4)	0.01949(13)	0.0310(5)
C29	0.74763(8)	−0.1493(4)	0.07433(13)	0.0326(5)
H29	0.7284	−0.2846	0.0611	0.039*
C30	0.87169(9)	0.4381(4)	0.01077(14)	0.0345(5)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H30A	0.8839	0.5021	−0.0372	0.041*
H30B	0.8497	0.5548	0.0307	0.041*
C31	0.94114(9)	0.6111(4)	0.09679(14)	0.0369(6)
H31A	0.9176	0.7158	0.1188	0.044*
H31B	0.9516	0.6852	0.0491	0.044*
C32	0.98713(10)	0.5700(4)	0.15906(14)	0.0425(6)
H32A	1.0043	0.7183	0.1727	0.051*
H32B	0.9761	0.5085	0.2083	0.051*
C33	0.99652(9)	0.2021(4)	0.10941(14)	0.0378(6)
H33A	0.9849	0.1319	0.1568	0.045*
H33B	1.0205	0.0945	0.0897	0.045*
C34	0.95193(8)	0.2378(4)	0.04506(13)	0.0331(5)
H34A	0.9635	0.3032	−0.0032	0.040*
H34B	0.9355	0.0885	0.0303	0.040*

Acknowledgements: We gratefully acknowledge support by Scientific and Technological Innovation Project of Sichuan (2017063); University Innovation and Entrepreneurship Training Program of China (201710634055; 201710634075).

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