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Crystal structure of (*S*)-1-(5-(anthracen-9-yl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)propan-1-one, C₂₆H₂₂N₂O

Table 1: Data collection and handling.

Crystal:	Prism, yellow
Size:	0.30 × 0.20 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
$\theta_{\max}$, completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	16967, 4302, 0.032
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3502
$N(\text{param})_{\text{refined}}$:	263
Programs:	Bruker programs [1], SHELX [2]

Source of materials

The title compound were synthesized by using previously reported protocol [3, 4]. A mixture of acetophenone (1.2 g, 9.9 mmol), 9-anthraldehyde (2.06 g, 9.9 mmol), and 3 M of aqueous sodium hydroxide (6 mL) in ethanol (20 mL) was stirred at room temperature for 8 h. The resulting solid was filtered to afford 3-(anthracen-9-yl)-1-phenylprop-2-en-1-one (chalcone), which was used without further purification. Then chalcone (1.2 g) and 3.5 g of an aqueous solution of hydrazine (80%) were dissolved in 20 mL of propionic acid. The mixture was then stirred at 120 °C for 5 h, and the resulting solution was cooled to room temperature and poured into ice water slowly. The crude product was collected by filtration and recrystallized from ethyl acetate to give pure product as yellow shaped crystals prism: 0.71 g, yield: 48.2%. Crystals were obtained by slow evaporation from methanol or ethanol at room temperature.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Anthracene derivatives have been playing an important role in the development of material chemistry [5–7], due to their excellent optical-physical properties [8, 9]. The title compound crystalizes in the orthorhombic and non-centrosymmetric space group *Pca*2₁, with one independent molecule in the asymmetric unit. The molecule shows

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Abstract

C₂₆H₂₂N₂O, orthorhombic, *Pca*2₁ (no. 29), $a = 22.8108(10)$ Å, $b = 9.8328(5)$ Å, $c = 8.7361(3)$ Å, $V = 1959.45(15)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0380$, $wR_{\text{ref}}(F^2) = 0.0853$, $T = 296(2)$ K.

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

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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	0.55088(6)	0.36772(15)	0.3663(2)	0.0551(4)
N1	0.59179(6)	0.54488(17)	0.48472(19)	0.0401(4)
N2	0.64092(6)	0.60582(16)	0.5498(2)	0.0403(4)
C1	0.31521(9)	0.5039(3)	0.4510(3)	0.0530(6)
H1	0.2763	0.4779	0.4623	0.064*
C2	0.32933(9)	0.6057(2)	0.3558(3)	0.0505(6)
H6	0.3000	0.6476	0.2989	0.061*
C3	0.38881(8)	0.6513(2)	0.3398(2)	0.0398(5)
C4	0.43351(8)	0.59116(19)	0.4338(2)	0.0364(4)
C5	0.49121(8)	0.64482(19)	0.4290(2)	0.0346(4)
C6	0.53561(8)	0.59865(19)	0.5479(2)	0.0379(4)
H20	0.5175	0.5275	0.6107	0.045*
C7	0.55791(8)	0.7119(2)	0.6547(2)	0.0422(5)
H14	0.5447	0.8006	0.6204	0.051*
H13	0.5448	0.6974	0.7590	0.051*
C8	0.62343(8)	0.6992(2)	0.6425(2)	0.0384(4)
C9	0.66533(8)	0.7843(2)	0.7266(2)	0.0407(5)
C10	0.72473(9)	0.7533(2)	0.7305(3)	0.0547(6)
H12	0.7388	0.6793	0.6755	0.066*
C11	0.76290(10)	0.8313(3)	0.8153(3)	0.0657(7)
H9	0.8025	0.8087	0.8186	0.079*
C12	0.74290(12)	0.9428(3)	0.8953(3)	0.0671(7)
H2	0.7689	0.9955	0.9517	0.081*
C13	0.53033(11)	0.9518(2)	0.1021(3)	0.0583(6)
H3	0.5390	1.0182	0.0298	0.070*
C14	0.47572(11)	0.9005(2)	0.1118(3)	0.0544(6)
H4	0.4470	0.9318	0.0450	0.065*
C15	0.46086(9)	0.7997(2)	0.2218(2)	0.0411(5)
C16	0.40369(9)	0.7520(2)	0.2366(3)	0.0456(5)
H5	0.3746	0.7891	0.1749	0.055*
C17	0.35954(9)	0.4366(2)	0.5340(3)	0.0504(5)
H7	0.3499	0.3622	0.5946	0.060*
C18	0.41620(8)	0.4787(2)	0.5268(2)	0.0431(5)
H8	0.4444	0.4331	0.5839	0.052*
C19	0.68446(12)	0.9758(3)	0.8916(3)	0.0661(7)
H10	0.6708	1.0513	0.9450	0.079*
C20	0.64577(10)	0.8962(2)	0.8081(3)	0.0536(6)
H11	0.6061	0.9183	0.8069	0.064*
C21	0.59545(9)	0.4259(2)	0.4060(2)	0.0418(5)
C22	0.65663(9)	0.3746(2)	0.3703(3)	0.0489(5)
H18	0.6778	0.4437	0.3136	0.059*
H19	0.6775	0.3584	0.4653	0.059*
C23	0.65507(12)	0.2444(3)	0.2775(4)	0.0711(8)
H15	0.6338	0.1761	0.3329	0.107*
H16	0.6944	0.2136	0.2594	0.107*
H17	0.6360	0.2612	0.1814	0.107*
C24	0.50527(8)	0.74748(19)	0.3226(2)	0.0361(4)
C25	0.56251(9)	0.8059(2)	0.3072(2)	0.0428(5)
H21	0.5924	0.7758	0.3710	0.051*
C26	0.57434(10)	0.9039(2)	0.2024(3)	0.0522(6)
H22	0.6119	0.9401	0.1964	0.063*

a twisted structure, in which the pyrazoline ring and anthracene ring are approximately perpendicular (86.2°). The *S*-enantiomers are linked by weak CH···O hydrogen bond (C···O = 3.188(1) Å) to construct a helical chain motif, which are in accord with the literature [10]; the adjacent chains with opposite chirality associate alternately along the *a* axis to form the overall 3D structure.

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