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Synthesis and crystal structure of the novel chiral acetyl-3-thiophene-5-(9-anthryl)-2-pyrazoline, $C_{23}H_{18}N_2OS$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size	0.20 × 0.20 × 0.15 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.19 mm ⁻¹
Diffractometer, scan mode:	Enraf Nonius TurboCAD4, ω
$\theta_{\max}$, completeness:	25.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3799, 3418, 0.046
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2373
$N(\text{param})_{\text{refined}}$:	247
Programs:	CAD4 [1, 2], SHELX [3], Diamond [4]

list of the atoms including atomic coordinates and displacement parameters.

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Abstract

$C_{23}H_{18}Cl_4N_2OS$, orthorhombic, $P2_12_1$ (no. 19), $a = 16.872(3)$ Å, $b = 10.414(2)$ Å, $c = 10.589(2)$ Å, $V = 1860.5(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0588$, $wR_{\text{ref}}(F^2) = 0.1464$, $T = 293$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the

Source of material

Acetyl-3-thiophene-5-(9-anthryl)-2-pyrazoline (ATAP) was prepared by a reported method [5, 6], in 80% yield. An ATAP single crystal was grown from ethyl acetate solution (10 mL) by slow evaporation at room temperature resulting in needle crystals after three days.

Experimental details

The hydrogen atoms were placed in calculated positions and refined using a riding model, with $C-H = 0.96$ Å (methylene) with $U_{\text{iso}}(H) = 1.2 U_{\text{eq}}(C)$.

Comment

Pyrazoline is a heterocyclic aromatic compound identified by a five-member ring system featuring three carbon atoms and two nitrogen atoms demonstrating strong blue fluorescence and good candidates in hole-transporters [7, 8]. Employing crystal engineering rules, pyrazoline derivatives have extensively employed as host materials

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
S	0.93740 (16)	0.45333 (15)	0.19170 (9)	0.0508 (5)
O	0.6173 (4)	0.4287 (4)	0.5315 (2)	0.0615 (12)
N1	0.7410 (4)	0.3942 (4)	0.4262 (3)	0.0395 (12)
N2	0.8068 (4)	0.4369 (4)	0.3582 (3)	0.0407 (11)
C1	0.7081 (5)	0.0807 (5)	0.5277 (3)	0.0385 (13)
C2	0.8094 (6)	0.0897 (6)	0.5845 (4)	0.0528 (16)
H2B	0.8712	0.1526	0.5792	0.063*
C3	0.8167 (7)	0.0076 (7)	0.6465 (4)	0.065 (2)
H3A	0.8825	0.0167	0.6833	0.078*
C4	0.7281 (8)	−0.0898 (7)	0.6561 (4)	0.073 (2)
H4A	0.7357	−0.1448	0.6988	0.088*
C5	0.6317 (7)	−0.1046 (6)	0.6040 (4)	0.0607 (19)
H5A	0.5729	−0.1696	0.6110	0.073*
C6	0.6188 (6)	−0.0208 (5)	0.5377 (4)	0.0469 (15)
C7	0.5203 (6)	−0.0370 (6)	0.4829 (4)	0.0540 (17)
H7A	0.4604	−0.1009	0.4911	0.065*
C8	0.5089 (5)	0.0400 (6)	0.4159 (3)	0.0447 (14)
C9	0.4101 (6)	0.0184 (6)	0.3592 (4)	0.0587 (18)
H9A	0.3520	−0.0471	0.3672	0.070*
C10	0.3994 (6)	0.0916 (7)	0.2940 (4)	0.0635 (19)
H10A	0.3338	0.0771	0.2577	0.076*
C11	0.4879 (6)	0.1897 (7)	0.2811 (4)	0.0573 (18)
H11A	0.4813	0.2391	0.2357	0.069*
C12	0.5828 (5)	0.2135 (6)	0.3340 (3)	0.0455 (15)
H12A	0.6403	0.2786	0.3235	0.055*
C13	0.5979 (5)	0.1424 (5)	0.4053 (3)	0.0372 (13)
C14	0.6937 (5)	0.1645 (5)	0.4633 (3)	0.0375 (13)
C15	0.7908 (5)	0.2717 (5)	0.4557 (3)	0.0406 (14)
H15A	0.8282	0.2863	0.5083	0.049*
C16	0.9009 (6)	0.2461 (6)	0.3981 (3)	0.0495 (16)
H16A	0.9828	0.2444	0.4255	0.059*
H16B	0.8887	0.1666	0.3706	0.059*
C17	0.8940 (5)	0.3553 (5)	0.3416 (3)	0.0380 (13)
C18	0.9768 (5)	0.3645 (5)	0.2727 (3)	0.0409 (14)
C19	1.0905 (6)	0.3020 (6)	0.2620 (4)	0.0542 (16)
H19A	1.1261	0.2470	0.2990	0.065*
C20	1.1475 (6)	0.3310 (6)	0.1881 (4)	0.0597 (18)
H20A	1.2265	0.2994	0.1717	0.072*
C21	1.0746 (7)	0.4094 (6)	0.1440 (4)	0.0559 (17)
H21A	1.0967	0.4364	0.0933	0.067*
C22	0.6640 (6)	0.4689 (6)	0.4698 (4)	0.0450 (14)
C23	0.6379 (7)	0.5997 (6)	0.4395 (4)	0.066 (2)
H23A	0.6304	0.5977	0.3828	0.099*
H23B	0.7072	0.6546	0.4543	0.099*
H23C	0.5592	0.6305	0.4621	0.099*

to modulate their luminescence characteristics, which in turn have potential applications in the fields of light-emitting diode owing to their promising optoelectronic applications [9–11]. Furthermore, pyrazoline containing compounds has been extensively reported exhibiting remarkable bioactivities [12–15].

The title compound crystallizes in the orthorhombic system with space group $P2_12_12_1$. In the structure, the homochiral molecules associate through weak C16–H16...O hydrogen bonds forming a homochiral chain. The two neighboring anthracene rings form an arrangement with a centroid–centroid distance and an interplanar separation of 6.703 and 6.116 Å indicating no π – π interaction while there is a weak π – π interaction between the anthracene ring of one molecule and the pyrazoline ring of a neighboring molecule with a centroid–centroid distance of 3.819 Å and an interplanar separation of 3.688 Å. Additionally, another hydrogen bond (C–H...N) links molecules to form another homochiral chain. The two chains are stacked in a parallel fashion.

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