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Crystal structure of (*E*)-1-(benzo[*d*]thiazol-2-yl)-*N*-(4,5-dihydropyren-2-yl)methanimine, $C_{24}H_{16}N_2S$

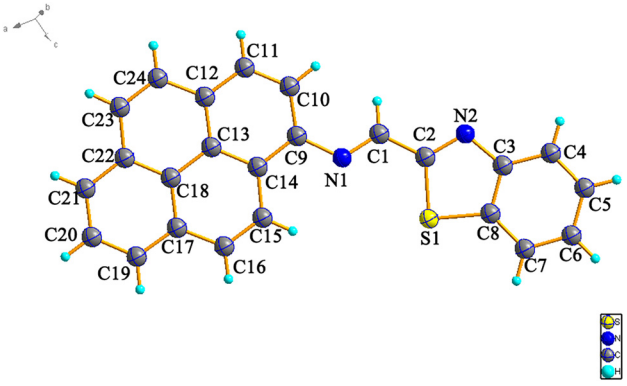

Table 1: Data collection and handling.

Crystal:	Orange block
Size:	0.28 × 0.18 × 0.16 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.20 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, 98 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7172, 2959, 0.038
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2384
$N(param)_{refined}$:	244
Programs:	SHELX [1, 2], Olex2 [3], Diamond [4]

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Abstract

$C_{24}H_{16}N_2S$, monoclinic, $P2_1/n$ (no. 14), a = 18.443(2) Å, b = 4.0161(6) Å, c = 23.396(4) Å, β = 99.246(6)°, V = 1710.4(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0589, $wR_{ref}(F^2)$ = 0.1173, T = 273.15 K.

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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

Under nitrogen protection, 1-aminopyrene (0.44 g, 2 mmol) and benzothiophen-2-formaldehyde (0.33 g, 2 mmol) were added to 100 mL round-bottomed flask, 50 mL anhydrous dichloromethane was added, and the mixture was stirred at 55 °C for 72 h. After the reaction, the reaction liquid was cooled to room temperature, the reaction liquid was filtered under reduced pressure, the solid was washed with anhydrous ethanol for three times, and the vacuum drying was performed. The target product (*E*)-1-(benzo[*d*]thiazol-2-yl)-*N*-(4,5-dihydropyren-2-yl) methanimine was obtained as 0.51 g of an orange powder with a yield of 70.8 %. The resulting product is dissolved in a mixture of dichloromethane and ethanol, left at room temperature, to grow orange crystals after a few days.

2 Experimental details

SADABS [1] was applied for absorption correction and the structure was solved and refined to convergence using the SHELXL-2014 [2] and OLEX2 programs [3]. All hydrogen atoms were positioned geometrically, with the d(C–H) = 0.97–0.99 Å, U_{iso}(H) = 1.2 times U_{eq}(C) and U_{iso}(H) = 1.5 times U_{eq}(O).

3 Comment

In recent years, a series of novel photosensitizers (PSs) with aggregation-induced emission (AIE) characteristics have attracted wide attention in the field of phototherapy [5–7], but its development remains a big challenge. Especially, planar AIE molecules, which are in the polymeric or solid state, excited-state double-bond reorganization (ESDBR) [8] is restricted, which enables dense emission of planar photons, and this class of molecules can produce type I ROS very well [9], which

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.53512 (15)	0.7768 (7)	0.61409 (12)	0.0415 (7)
H1	0.5175	0.8800	0.5790	0.050*
C2	0.49878 (14)	0.8341 (7)	0.66366 (11)	0.0359 (6)
C3	0.41432 (13)	0.9889 (6)	0.71431 (11)	0.0347 (6)
C4	0.34881 (14)	1.1250 (7)	0.72654 (13)	0.0447 (7)
H4	0.3156	1.2238	0.6973	0.054*
C5	0.33389 (15)	1.1117 (7)	0.78186 (14)	0.0471 (8)
H5	0.2906	1.2040	0.7902	0.057*
C6	0.38256 (16)	0.9622 (7)	0.82551 (13)	0.0474 (8)
H6	0.3711	0.9538	0.8628	0.057*
C7	0.44727 (15)	0.8263 (7)	0.81505 (12)	0.0427 (7)
H7	0.4798	0.7276	0.8447	0.051*
C8	0.46294 (13)	0.8399 (6)	0.75885 (11)	0.0345 (6)
C9	0.62540 (13)	0.5174 (6)	0.56995 (11)	0.0321 (6)
C10	0.59794 (14)	0.6126 (7)	0.51295 (11)	0.0388 (7)
H10	0.5541	0.7310	0.5055	0.047*
C11	0.63429 (14)	0.5351 (7)	0.46796 (11)	0.0396 (7)
H11	0.6147	0.6017	0.4306	0.048*
C12	0.70001 (14)	0.3584 (6)	0.47728 (11)	0.0347 (6)
C13	0.72933 (13)	0.2585 (6)	0.53466 (10)	0.0297 (6)
C14	0.69165 (13)	0.3371 (6)	0.58144 (10)	0.0319 (6)
C15	0.72276 (14)	0.2275 (7)	0.63840 (11)	0.0372 (7)
H15	0.6983	0.2736	0.6693	0.045*
C16	0.78673 (14)	0.0590 (7)	0.64816 (12)	0.0404 (7)
H16	0.8052	−0.0097	0.6856	0.048*
C17	0.82707 (14)	−0.0171 (6)	0.60247 (12)	0.0357 (6)
C18	0.79745 (13)	0.0835 (6)	0.54536 (11)	0.0326 (6)
C19	0.89386 (15)	−0.1870 (7)	0.61143 (13)	0.0459 (7)
H19	0.9134	−0.2585	0.6485	0.055*
C20	0.93122 (16)	−0.2503 (8)	0.56618 (15)	0.0532 (8)
H20	0.9763	−0.3590	0.5732	0.064*
C21	0.90270 (16)	−0.1548 (8)	0.51064 (14)	0.0504 (8)
H21	0.9288	−0.1994	0.4806	0.061*
C22	0.83527 (15)	0.0080 (7)	0.49885 (12)	0.0399 (7)
C23	0.80299 (16)	0.1053 (7)	0.44152 (13)	0.0464 (8)
H23	0.8269	0.0535	0.4106	0.056*
C24	0.73885 (16)	0.2700 (7)	0.43149 (12)	0.0431 (7)
H24	0.7192	0.3280	0.3937	0.052*
N1	0.59052 (11)	0.5881 (6)	0.61799 (9)	0.0368 (5)
N2	0.43606 (12)	0.9846 (6)	0.66046 (10)	0.0412 (6)
S1	0.53840 (4)	0.68841 (19)	0.73166 (3)	0.0401 (2)

provides a new idea for the development of new photosensitizers. Here, we report the crystal structure of (*E*)-1-(benzo[*d*]thiazol-2-yl)-*N*-(4,5-dihydropyren-2-yl)methanimine. The whole molecule is a planar molecule, forming a large conjugated system. But the molecules arrange interleaved. The π–π packing (π–π distance is 4.016 Å) is reduced, the molecular orbital overlap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) is reduced, and the occurrence of aggregation-caused quenching (ACQ) effect is reduced. As the crystal structure, the bond length of C1–N1 is 1.264(3) Å, which shows a typical C–N double bond, and pyrene group is the electron donor, and thiazole ring is the electron acceptor, forming a D–π–A structure molecule, which is a typical molecular structure characteristic of AIE. Therefore it will provide a good new design strategy for the development of planar AIE photosensitizer molecules.

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

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