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Crystal structure of 1*H*-indole-5-carboxylic acid – 4,4'-bipyridine (2/1), C₁₄H₁₁N₂O₂

Table 1: Crystal collection and handling.

Crystal:	Block, clear light yellow
Size:	0.31 × 0.24 × 0.21 mm
Wavelength:	Mo K α radiation (λ = 0.71073 Å)
μ :	0.092 mm ⁻¹
Diffraction, scan mode:	Xcalibur, Φ and ω -scans
$\theta_{\max}$, completeness:	27.0°, 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9030, 5086, 0.0284
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 0.1354
$N(\text{param})_{\text{refined}}$:	327
Programs:	CrysAlis ^{PRO} [1], OLEX2 [2], SHELX [3], Diamond [4]

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Abstract

C₁₄H₁₁N₂O₂, triclinic, $P\bar{1}$ (no. 2), a = 7.8749(6) Å, b = 9.6746(6) Å, c = 16.0818(12) Å, α = 78.200(6)°, β = 83.007(6)°, γ = 85.035(6)°, V = 1188.00(15) Å³, Z = 4, $R_{\text{gt}}(F)$ = 0.0638, $wR_{\text{ref}}(F^2)$ = 0.1712, T = 295.42(10) K.

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The asymmetric unit of the title 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.

Source of material

For this compound, a mixture of indole-5-carboxylic acid (0.1 mmol), 4,4'-bipyridine (0.1 mmol), H₂O (10 mL) and methanol 2 mL was stirred for 20 min and then sealed in a 25 mL Teflon-lined stainless steel autoclave and heated at 140 °C for 60 h. Colorless stick crystals of the title compound

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	1.2817(2)	0.4798(2)	0.01026(12)	0.0609(6)
H1	1.365557	0.516932	−0.017953	0.091
O2	1.4740(2)	0.4014(2)	0.10152(12)	0.0519(5)
O3	1.4475(2)	0.33915(19)	0.39351(12)	0.0515(5)
O4	1.2937(3)	0.48472(19)	0.46853(13)	0.0636(6)
H4	1.265000	0.409837	0.499022	0.095
N1	0.8036(3)	0.2603(2)	0.34544(14)	0.0480(6)
H1	0.693524	0.263015	0.348832	0.058
N2	0.8588(3)	0.7020(2)	0.40957(14)	0.0487(6)
N3	1.2540(3)	0.9682(3)	−0.00457(17)	0.0673(8)
N4	1.6039(3)	0.9505(2)	0.18053(16)	0.0567(7)
H4	1.653783	0.967973	0.129213	0.068
C1	0.8995(4)	0.2160(3)	0.41208(18)	0.0497(7)
H1	0.854995	0.184828	0.468458	0.060
C2	1.0676(3)	0.2238(3)	0.38492(16)	0.0446(7)
H2	1.158276	0.198287	0.418184	0.054
C3	1.0797(3)	0.2785(2)	0.29535(16)	0.0355(6)
C4	1.2144(3)	0.3165(2)	0.23257(15)	0.0346(6)
H4	1.326831	0.304683	0.246279	0.042
C5	1.1801(3)	0.3718(2)	0.14994(16)	0.0351(6)
C6	1.3210(3)	0.4195(3)	0.08439(17)	0.0386(6)
C7	1.0109(3)	0.3879(3)	0.12873(17)	0.0424(7)
H7	0.990221	0.423511	0.072392	0.051
C8	0.8757(3)	0.3522(3)	0.18930(17)	0.0451(7)
H8	0.763865	0.363037	0.174857	0.054
C9	0.9103(3)	0.2998(2)	0.27241(16)	0.0370(6)
C10	1.4001(3)	0.4586(3)	0.40370(17)	0.0428(7)
C11	1.4527(3)	0.5880(3)	0.34266(16)	0.0403(6)
C12	1.5289(3)	0.5756(3)	0.26147(17)	0.0468(7)
H12	1.543652	0.486568	0.247151	0.056

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C13	1.5828(4)	0.6904(3)	0.20210(17)	0.0511(8)
H13	1.632730	0.680852	0.147938	0.061
C14	1.5603(3)	0.8211(3)	0.22565(17)	0.0440(7)
C15	1.5547(4)	1.0478(3)	0.2309(2)	0.0672(10)
H15	1.570674	1.144097	0.214578	0.081
C16	1.4798(4)	0.9849(3)	0.3074(2)	0.0681(10)
H16	1.435099	1.028943	0.352340	0.082
C17	1.4823(3)	0.8381(3)	0.30633(18)	0.0470(7)
C18	1.4282(3)	0.7190(3)	0.36531(17)	0.0487(7)
H18	1.376218	0.727835	0.419250	0.058
C19	0.9319(4)	0.6176(3)	0.35833(18)	0.0529(8)
H19	0.927562	0.520446	0.377553	0.063
C20	1.0132(4)	0.6652(3)	0.27889(18)	0.0519(8)
H20	1.062338	0.600977	0.245684	0.062
C21	1.0224(3)	0.8084(3)	0.24795(17)	0.0387(6)
C22	0.9509(4)	0.8958(3)	0.30212(18)	0.0538(8)
H22	0.957141	0.993265	0.285425	0.065
C23	0.8709(4)	0.8396(3)	0.38043(19)	0.0601(9)
H23	0.821963	0.901442	0.415288	0.072
C24	1.1031(3)	0.8643(3)	0.16101(17)	0.0413(6)
C25	1.1024(5)	0.7918(3)	0.0958(2)	0.0729(11)
H25	1.051484	0.705823	0.105963	0.087
C26	1.1775(5)	0.8473(4)	0.0155(2)	0.0854(13)
H26	1.174380	0.796697	−0.027505	0.102
C27	1.2524(5)	1.0362(3)	0.0581(2)	0.0768(11)
H27	1.304167	1.121957	0.046121	0.092
C28	1.1801(4)	0.9904(3)	0.1402(2)	0.0669(10)
H28	1.183350	1.044620	0.181523	0.080

were obtained, which were washed with water and dried in air with a 73% yield.

Experimental details

The aromatic CH as well as the OH groups were idealized and introduced in the structural model using rigid groups (AFIX 43 and 83 options of SHELX program system), with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$, respectively.

Comment

Cocrystals are of general interest [6] and especially of those with 4,4'-bipyridine and a benzoic acid are a subject of a recent study [7].

There are two acid molecules and one 4,4'-bipyridine molecule in the asymmetric unit (*cf.* the figure). Bond lengths and angles are in the expected ranges. $\text{NH} \cdots \text{O}$ and $\text{NH} \cdots \text{N}$ hydrogen bonds connect the molecules in the title crystal structure.

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