Wenxiang Wang* and Chao Zhu

The crystal structure of 4-((2-hydroxynaphthalen-1-yl)(pyrrolidin-1-yl)methyl)benzonitrile, $C_{22}H_{20}N_2O$

Table 1: Data collection and handling.

Crystal:	Colorless prism
Size:	0.38 × 0.18 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.07 mm ⁻¹
Diffractometer, scan mode:	Rigaku SCXmini, ω
$\theta_{\max}$, completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	18,320, 2195, 0.083
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1493
$N(\text{param})_{\text{refined}}$:	227
Programs:	CrystalClear [1], SHELX [2–4], Diamond [5]

of the atoms including atomic coordinates and displacement parameters.

Source of material

A dry 50 ml flask was charged with 4-formylbenzonitrile (10 mmol), naphthalen-2-ol (10 mmol), and pyrrolidine (10 mmol). The mixture was stirred at 100 °C for 10 h and then added ethanol (15 ml). After heating under reflux for 30 min, the precipitate was filtrated out and washed with ethanol for 2–3 times and purified by recrystallization from dichloromethane to give the target material. Crystals of the title compound were obtained by slow evaporation from a mixture of methanol and DMF.

Experimental details

All hydrogen atoms were calculated geometrically and with C–H distances ranging from 0.93 to 0.98 Å. $C_{\text{aryl}}\text{--H} = 0.93$ Å, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. $C_{\text{pyrrolidine}}\text{--H} = 0.96$ Å, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$. O–H = 0.82 Å with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. The absolute structure can not be established [5].

Comment

We are interested in the dielectric-ferroelectric materials, including organic ligands [6], metal-organic coordination

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Abstract

$C_{22}H_{20}N_2O$, orthorhombic, $Pna2_1$ (no. 33), $a = 11.677(2)$ Å, $b = 13.999(3)$ Å, $c = 11.171(2)$ Å, $V = 1826.2(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0521$, $wR_{\text{ref}}(F^2) = 0.1078$, $T = 293$ K.

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

*Corresponding author: Wenxiang Wang, Jiangsu Vocational Institute of Architectural Technology, Xuzhou 221116, People's Republic of China, E-mail: wxwang_1109@163.com. <https://orcid.org/0000-0001-7297-3387>

Chao Zhu, School of Chemical Engineering, Yunnan Open University, Kunming 650500, People's Republic of China. <https://orcid.org/0000-0002-8031-2551>

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}
C1	0.9407 (2)	0.0853 (2)	0.2172 (3)	0.0417 (7)
H1	0.9262	0.0483	0.2901	0.050*
C2	1.0507 (2)	0.0481 (2)	0.1604 (3)	0.0419 (7)
C3	1.1225 (3)	0.1072 (2)	0.0954 (3)	0.0512 (8)
C4	1.2230 (3)	0.0712 (3)	0.0412 (4)	0.0609 (10)
H4	1.2701	0.1121	−0.0020	0.073*
C5	1.2512 (3)	−0.0215 (3)	0.0515 (4)	0.0641 (10)
H5	1.3184	−0.0436	0.0163	0.077*
C6	1.1803 (3)	−0.0862 (3)	0.1150 (3)	0.0539 (9)
C7	1.0777 (3)	−0.0513 (2)	0.1686 (3)	0.0458 (8)
C8	1.0065 (3)	−0.1187 (2)	0.2273 (3)	0.0562 (9)
H8	0.9378	−0.0983	0.2608	0.067*
C9	1.0363 (4)	−0.2121 (3)	0.2358 (4)	0.0722 (12)
H9	0.9884	−0.2545	0.2757	0.087*
C10	1.1387 (4)	−0.2452 (3)	0.1850 (4)	0.0783 (13)
H10	1.1589	−0.3093	0.1921	0.094*
C11	1.2086 (4)	−0.1835 (3)	0.1253 (4)	0.0697 (11)
H11	1.2759	−0.2060	0.0908	0.084*
C12	0.8381 (2)	0.0737 (2)	0.1346 (3)	0.0378 (7)
C13	0.7371 (2)	0.0343 (2)	0.1760 (3)	0.0450 (8)
H13	0.7337	0.0106	0.2536	0.054*
C14	0.6411 (3)	0.0296 (2)	0.1044 (3)	0.0453 (8)
H14	0.5735	0.0035	0.1338	0.054*
C15	0.6461 (3)	0.0636 (2)	−0.0107 (3)	0.0415 (7)
C16	0.7470 (3)	0.1015 (3)	−0.0551 (3)	0.0534 (9)
H16	0.7504	0.1240	−0.1334	0.064*
C17	0.8423 (3)	0.1057 (2)	0.0170 (3)	0.0520 (9)
H17	0.9104	0.1303	−0.0133	0.062*
C18	0.5450 (3)	0.0616 (2)	−0.0855 (3)	0.0476 (8)
C19	1.0281 (3)	0.2010 (3)	0.3569 (3)	0.0546 (9)
H19A	1.1078	0.1899	0.3368	0.066*
H19B	1.0064	0.1585	0.4216	0.066*
C20	1.0083 (3)	0.3041 (3)	0.3911 (4)	0.0678 (10)
H20A	1.0652	0.3452	0.3543	0.081*
H20B	1.0117	0.3121	0.4773	0.081*
C21	0.8885 (3)	0.3270 (3)	0.3439 (4)	0.0722 (12)
H21A	0.8382	0.3460	0.4088	0.087*
H21B	0.8916	0.3783	0.2855	0.087*
C22	0.8468 (3)	0.2351 (2)	0.2863 (3)	0.0542 (9)
H22A	0.8035	0.1968	0.3428	0.065*
H22B	0.7994	0.2483	0.2169	0.065*
N1	0.9536 (2)	0.18689 (17)	0.2516 (2)	0.0435 (7)
N2	0.4658 (3)	0.0601 (2)	−0.1441 (3)	0.0702 (9)
O1	1.10309 (19)	0.20191 (16)	0.0794 (3)	0.0652 (7)
H1A	1.0490	0.2187	0.1212	0.098*

compounds and organic-inorganic hybrids [7]. Because of their wide distribution in bioactive molecules [8] and pharmaceuticals, [9] there is considerable interest in the development of effective methods for the synthesis of compounds derived from naphthalen-2-ol [10]. Recent

studies have revealed that a betti-base organic compound was obtained, we report here.

There is one molecule in the asymmetric unit, as can be seen in the figure. All bond lengths are in normal ranges [11]. The dihedral angle between the planes of the naphthyl ring and of the phenyl ring is 72.91(8)°. Strong intramolecular O–H⋯N hydrogen bonding [O1–H1A = 0.82 Å, H1A⋯N1 = 1.89 Å, O1–N1 = 2.606(4) Å, O1–H1A⋯N1 = 146°] together with van-der-Waals interactions stabilize the molecular conformation [12].

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References

1. Rigaku: *CrystalClear-SM Expert*; Rigaku Corporation: Tokyo, Japan, 2005.
2. Sheldrick G. M. SHELXT – integrated space-group and crystal-structure determination. *Acta Crystallogr.* 2015, *A71*, 3–8.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Parsons S., Flack H. D., Wagner T. Use of intensity quotients and differences in absolute structure refinement. *Acta Crystallogr.* 2013, *B69*, 249–259.
5. Brandenburg K. *DIAMOND*. Visual Crystal Structure Information 44System. Ver. 4.0; Crystal Impact: Bonn, Germany, 2015.
6. Tang Y., Li P., Liao W., Shi P., You Y., Xiong R. Multiaxial molecular ferroelectric thin films bring light to practical applications. *J. Am. Chem. Soc.* 2018, *140*, 8051–8059.
7. Liao W., Zhao D., Tang Y., Zhang Y., Li P., Shi P., Chen X., You Y., Xiong R. An organic-inorganic perovskite ferroelectric with large piezoelectric response. *Science* 2019, *363*, 1206–1210.
8. Betti M. General condensation reaction among naphthol, aldehyde, and amine. *Gazz. Chim. Ital.* 1900, *30*, 310–316.
9. Ma W., Chen F., Liu Y., He Y. M., Fan Q. H. Ruthenium catalyzed enantioselective hydrogenation of 1,8-naphthyridine derivatives. *Org. Lett.* 2016, *18*, 2730–2733.
10. Wang W., Zhao H. 1-[(Dimethylamino)(phenyl)methyl] naphthalen-2-ol. *Acta Crystallogr.* 2008, *E64*, o1900.

11. Jia G.-K., Chen X.-M., He F.-L., Chen X.-W., Wang Z.-C. Crystal structure of 2-(3,4-dimethylphenyl)-1,8-naphthyridine, $C_{16}H_{14}N_2$. *Z. Kristallogr. NCS* 2018, 233, 819–820.
12. Chen X.-Y., Zhao M.-M., Qian X., Hou S.-G. 4-[(Hydroxynaphthalen-1-yl)(morpholin-4-yl)methyl]benzonitrile. *Acta Crystallogr.* 2011, E67, o3484.