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The crystal structure of 1,2-bis(4-pyridyl)ethane - 4,4-dihydroxydiphenylmethane (1/1), C₂₅H₂₁N₂O₂

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.41 × 0.23 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Rigaku R-Axis RAPID, ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7912, 1833, 0.046
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1121
$N(\text{param})_{\text{refined}}$:	132
Programs:	RAPID-AUTO [1], SHELX [2, 3]

<https://doi.org/10.1515/ncrs-2021-0148>

Received April 18, 2021; accepted April 29, 2021;

published online May 13, 2021

Abstract

C₂₅H₂₁N₂O₂, monoclinic, $C2/c$ (no. 15), $a = 11.041(2)$ Å, $b = 7.859(2)$ Å, $c = 24.131(5)$ Å, $\beta = 95.26(3)^\circ$, $V = 2085.1(7)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0486$, $wR_{\text{ref}}(F^2) = 0.1402$, $T = 295$ K.

CCDC no.: 2078290

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound has been synthesized according to the following method: 0.2003 g (1.0 mmol) 4,4-dihydroxydiphenylmethane and 0.1842 g (1.0 mmol) 1,2-bis(4-pyridyl)ethane were successively added to 20 mL

methanol-water (v:v = 1:1). The solution was allowed to stand at room temperature for three days, colorless block crystals were obtained.

Experimental details

The structure was solved by direct methods with the SHELXS program. All H-atoms at C atoms were positioned with idealized geometry and refined isotropically ($U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$), using a riding model with C–H = 0.93 Å or 0.96 Å. H atoms attached to O atoms were found in a difference Fourier synthesis and were refined using a riding model, with the O–H distances fixed as initially found and with $U_{\text{iso}}(\text{H})$ values set at $1.5U_{\text{eq}}(\text{O})$.

Comment

Organic cocrystals, composed of two or more molecular and/or ionic compounds in a stoichiometric ratio, are crystalline or single-phase materials [4, 5]. Over the past decades, they have attracted wide attention and emerged as a promising research interest to construct functional materials due to their unique electrical, magnetic, and optical properties [6–8]. Crystallization is a typical self-assembly phenomenon [9]. The synergistic effect of those non-covalent bonding interactions between homomeric and heteromeric molecules governs recognition and assembly process [10–14]. The synthon that is formed

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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}
N1	0.68915 (17)	0.5103 (2)	0.56133 (9)	0.0827 (6)
O1	0.80659 (16)	0.7771 (2)	0.61794 (8)	0.1045 (6)
H1B	0.769426	0.699137	0.601436	0.157*
C1	0.6486 (2)	0.3846 (3)	0.59222 (10)	0.0889 (7)
H1A	0.659699	0.395780	0.630723	0.107*
C2	0.5922 (2)	0.2410 (3)	0.57102 (10)	0.0812 (7)
H2A	0.565853	0.158329	0.594726	0.097*
C3	0.57448 (18)	0.2197 (3)	0.51376 (9)	0.0687 (6)
C4	0.61564 (18)	0.3507 (3)	0.48175 (9)	0.0722 (6)
H4A	0.606149	0.342875	0.443136	0.087*
C5	0.6698 (2)	0.4905 (3)	0.50641 (11)	0.0773 (7)
H5A	0.694653	0.576915	0.483673	0.093*
C6	0.51960 (18)	0.0680 (3)	0.48763 (9)	0.0764 (6)
H6A	0.511212	0.067009	0.448926	0.092*
C7	0.7773 (3)	0.9987 (3)	0.68096 (11)	0.0930 (8)
H7A	0.858162	1.030358	0.679906	0.112*
C8	0.7024 (3)	1.0884 (3)	0.71386 (10)	0.0906 (8)
H8A	0.734620	1.179410	0.734986	0.109*
C9	0.5825 (2)	1.0465 (3)	0.71606 (9)	0.0811 (7)
C10	0.5384 (2)	0.9080 (3)	0.68516 (10)	0.0828 (7)
H10A	0.457515	0.876246	0.686172	0.099*
C11	0.6120 (2)	0.8153 (3)	0.65273 (9)	0.0787 (6)
H11A	0.580689	0.721214	0.632911	0.094*
C12	0.7308 (2)	0.8619 (3)	0.64976 (10)	0.0780 (6)
C13	0.500000	1.1501 (4)	0.750000	0.0995 (11)
H13A	0.450320	1.222249	0.725140	0.119*

between bisphenol and other moieties is one of the most exploited synthon for designing cocrystal [15–19].

The asymmetric unit of the title structure contains one half of a 4,4'-dihydroxydiphenylmethane molecule and one half of a 1,2-bis(4-pyridyl)ethane molecule (see the figure). Bond lengths and angles are within normal ranges. In the crystal structure of the title complex, O–H···N hydrogen interactions (O1···N1 = 2.759(6) Å; O1–H1B···N1 = 177.1°) between the 4,4'-dihydroxydiphenylmethane and 1,2-bis(4-pyridyl)ethane molecules lead to the formation of a chain along the *c* axis. Two pyridine groups of neighboring molecules, related by inversion symmetry are involved in a π – π interaction with a centroid-centroid distance of 3.78 Å forming a two-dimensional layer structure parallel to (100).

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: None declared.

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

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