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The crystal structure of (4-fluorophenyl)(5-(hydroxymethyl)furan-2-yl)methanol, C₁₂H₁₁FO₃

Abstract

C₁₂H₁₁FO₃, monoclinic, P₂₁/c (no. 14), a = 12.0648(9) Å, b = 8.3896(5) Å, c = 10.5727(9) Å, β = 104.204(8) °, V = 1037.44(14) Å³, Z = 4, Rgt(F) = 0.0614, wRref(F²) = 0.1516, 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 of the atoms including atomic coordinates and displacement parameters.

Source of materials

An amount of 5 mmol 5-hydroxymethylfurfural (HMF) was dissolved in anhydrous tetrahydrofuran (THF). The fluoro-Grignard reagent (4-fluorophenyl magnesium bromide, 12.5 mL, 1 mol/L) was added to the solution slowly at ice-water bath conditions. The mixture was then stirred for 30 min at room temperature. Subsequently, 0.5 mL saturated ammonium chloride solution was added, and stirred for 30 min. The solution was later extracted three times with ethyl acetate, and the organic phases were combined. The product was further purified by column chromatography (1:1 petroleum ether/ethyl acetate). Upon slow evaporation at room temperature, crystals were acquired after one week.

Experimental details

All H atoms were refined as riding atoms in their geometrically idealized positions, with d(C–H) = 0.93 Å and Ueq(H) = 1.2 Ueq(C).

Comment

HMF (Hydroxymethylfurfural) is considered as an important building block platform, because it can be obtained from direct transformation of fructose, glucose, sucrose, cellulose, and inulin [5, 6]. The functional groups of HMF, including C=O, C–O, and furan ring, allows this compound some flexibility in its catalytic conversions of multifunctional substrates and in the future of value-added chemicals and fuel component [5, 7]. For example, the synthesis of 2,5-diformylfuran (DFF) from selective oxidation of HMF is commercially important, because DFF is a versatile precursor
Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

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<tr>
<th></th>
<th>x</th>
<th>y</th>
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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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