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Ferrocenecarbaldehyde isonicotinyl hydrazide

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The chiral structure of ferrocenecarbaldehyde isonicotinyl hydrazide, [Fe(η^5-C_5H_5)(η^5-$C_{12}H_{10}N_3O$)], shows the molecule exhibits an *E* configuration, has a C═N bond length of 1.284(4) Å and an N–N bond length of 1.388(3) Å. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; ferrocenecarbaldehyde; isonicotinyl hydrazide

COMMENT

Schiff bases derived from acyhydrazine and their complexes exhibit strong antitumor and antivirus activities[1] and the incorporation of a ferrocenyl group can improve these properties.[2,3] Some ferrocene derivatives are excellent nonlinear optical materials[4] owing to their strong electron donor properties and behavior as an electron-flow bridge. Their interesting structural characteristics and wide-ranging applications are the impulse for our carrying out this aspect study. Figure 1 shows the chiral molecular structure of ferrocenecarbaldehyde isonicotinyl hydrazide, [Fe(η^5-C_5H_5)(η^5-$C_{12}H_{10}N_3O$)] (**1**). Similar to the structure of the 2-pyridylhydrazone of ferrocenecarbaldehyde,[5] the molecule exhibits an *E* configuration, has a C═N bond length of 1.284(4) Å and an N–N bond length of 1.388(3) Å, which are longer than in 2-pyridylhydrazone of ferrocenecarbaldehyde; the cyclopentadienyl rings are eclipsed with Fe–C distance of 2.021(4) to 2.048(4) Å, mean 2.036(4) Å. The cyclopentadienyl rings are essentially parallel. The pyridyl group is not coplanar with the cyclopentadienyl ring, but inclined at an angle of 3.76(21)° to it. The distances and angles involving the pyridyl ring are comparable to that of 2-pyridylhydrazone of ferrocenecarbaldehyde.[5] Through the strong intermolecular hydrogen bonding involving the pyridyl nitrogen and the NH group of isonicotinyl hydrazide (N(2)–H(2)···N(3A) 2.831(4) Å, A: $-x+1, y+1/2, -z+3/2$), a one-dimensional zigzag chain is formed (Fig. 2).

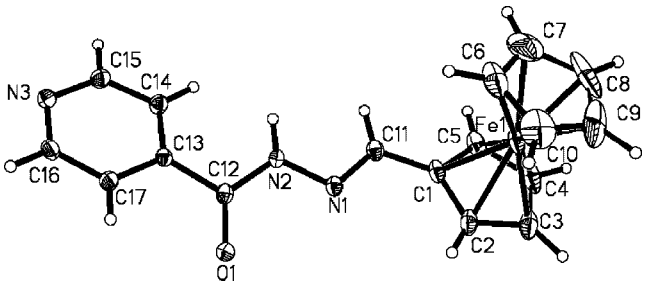

Figure 1. Molecular structure of [Fe(η^5-C_5H_5)(η^5-$C_{12}H_{10}N_3O$)]. Key geometric parameters: Fe1–C1 2.041(3), Fe1–C2 2.045(4), Fe1–C3 2.048(4), Fe1–C4 2.040(3), Fe1–C5 2.029(3), Fe1–C6 2.031(4), Fe1–C7 2.035(5), Fe1–C8 2.021(4), Fe1–C9 2.029(4), Fe1–C10 2.045(4), C11–N1 1.284(4), C12–N2 1.356(4), C12–O1 1.232(4), N1–N2 1.388(3) Å; C11–N1–N2 114.0(3), C12–N2–N1 120.7(2), N(2)–C12–O1 123.9(3), C13–C12–O1 121.6(3), C13–C12–N2 114.4(3)°.

EXPERIMENTAL

Samples of ferrocenecarbaldehyde (0.2 mmol), isonicotinyl hydrazide (0.2 mmol) and $Cu(Ac)_2 \cdot H_2O$ (0.1 mmol) were thoroughly mixed in a mortar with a pestle, and placed in thick-walled Pyrex tubes (*ca* 20 cm long). After addition of 2-butyl alcohol (2.5 ml), the tube was frozen with liquid

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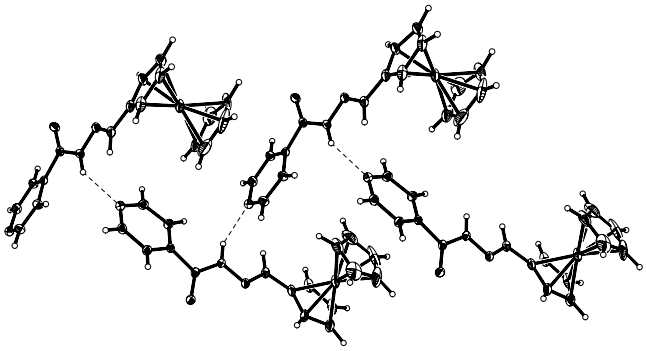

Figure 2. One-dimensional zigzag chain formed through intermolecular hydrogen bonding.

nitrogen, evacuated under vacuum and sealed with a torch. The tube was heated at 75 °C for 2 days to give red–brown block crystals. Yield: 35%. Anal. Calc. for $C_{17}H_{15}FeN_3O$: C, 61.23; H, 4.5; N, 12.61. Found: C, 61.40; H, 4.42; N, 12.56%. X-ray diffraction data were collected at 193(2) K on a Rigaku Mercury CCD diffractometer using graphite-monochromated Mo Kα radiation on a block 0.21 × 0.15 × 0.10 mm^3. Crystallographic data: $C_{17}H_{15}FeN_3O$, M = 333.17, orthorhombic, $P2_12_12_1$, a = 6.6243(8), b = 10.6477(13), c = 20.802(3) Å, V = 1467.2(3) Å^3, Z = 4, D = 1.508 Mg m^{-3}, 16 646 reflections collected, 3368 unique and 2931 $I > 2\sigma(I)$. R = 0.0455 (obs. data on F^2), wR = 0.0981 (all data), ρ_{max} = 0.316 e$^-$ Å^{-3}, Flack parameter 0.01(2). Programs used: SHELXTL97, ORTEP. CCDC deposition number: CCDC236668.

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