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Synthesis and crystal structure of 4-(2,4-dinitrophenoxy)benzaldehyde, C_{13}H_{8}N_{2}O_{6}

Abstract
C_{13}H_{8}N_{2}O_{6}, triclinic, \( P_1 \) (no. 2), \( a = 6.9561(5) \) Å, \( b = 7.3040(5) \) Å, \( c = 13.2883(8) \) Å, \( \alpha = 100.988(3) \)°, \( \beta = 95.557(3) \)°, \( \gamma = 107.424(3) \)°, \( V = 623.76(7) \) Å\(^3\), \( Z = 2 \), \( R_{\text{gt}}(F) = 0.0376 \), \( wR_{\text{ref}}(F^2) = 0.1008 \), \( T = 150(2) \) K.

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The molecular structure is shown in the Figure (showing 40% probability displacement ellipsoids). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material
4-Hydroxybenzaldehyde (122 mg, 10 mmol), anhydrous potassium carbonate (276 mg, 2 mmol), 2,4-dinitrofluorobenzene (186 mg, 10 mmol) and anhydrous dichloromethane (15 mL) were added to a 50 ml round flask. The mixture was stirred at room temperature for 2–3 h. After the reaction was complete, the reaction mixture was concentrated under reduced pressure, and the residue was purified with ethyl acetate–petroleum ether (1:2, v/v) as eluent by silica gel chromatography column to obtain a light yellow solid (195 mg, yield 68%). The product was dissolved in 80% ethanol and recrystallized to get colourless transparent blocks.

Experimental details
H atoms were included in calculated positions and refined using a riding model, with C–H distances constrained to 0.98 Å, respectively, and with \( U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C) \).

Comment
Thioredoxin reductase (TrxR) is one of the important targets for inhibiting tumor growth [5]. TrxR inhibitors...
The TrxR inhibitory activity of the title compound was determined by the TrxR activity detection kit. The results showed that the inhibition rate of the title compound against TrxR was 75.3(2.7) at 100 µM. Reports of the crystal structure are helpful to understand the mechanism of these 2,4-dinitrobenzene compounds and to develop more active 2,4-dinitrobenzene TrxR inhibitors.

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**References**