The crystal structure of 5,7-dinitropyrazolo[5,1-b]quinazolin-9(4H)-one, C_{10}H_{5}N_{5}O_{5}

Abstract

C_{10}H_{5}N_{5}O_{5}, monoclinic, \textit{P}2_1/c (no. 14), \(a = 10.9546(11)\) Å, \(b = 7.3433(8)\) Å, \(c = 13.2567(15)\) Å, \(β = 102.972(5)°\), \(V = 1039.19(19)\) Å\(^3\), \(Z = 4\), \(R_{gt}(F) = 0.0630\), \(wR_{ref}(F^2) = 0.1622\), \(T = 298\) K.

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

1 Source of materials

In a representative experiment 5,7-dinitropyrazolo[5,1-b]quinazolin-9(4H)-one (35.7 mg, 0.050 mmol) was dissolved in 8 mL of ethanol by heating the solution. The solution was then
filtered into a test tube and left standing at room temperature. After about 20 days colorless block crystals were obtained.

2 Experimental details

Hydrogen atoms attached to the C atoms were placed in calculated positions with d(C–H) = 0.93 Å.

3 Comment

Many heterocyclic compounds containing pyrazole residues showed potential biological activities and some of them had been employed in medicine [4]. 4H-pyrazolo[5,1-b]quinazolin-9-one and its derivatives are important N-containing tricyclic compounds with unique biological properties, which have been investigated in detail [4–8].

In the title crystal structure all of the bond distances and angles are in the normal range and the molecule is flat [9, 10] (upper part of the Figure) 5,7-dinitropyrazolo[5,1-b]quinazolin-9(4H)-one creates a dimer by the pi–pi contact from the aryl moieties with C–Cg = 3.354–3.384 Å, here both molecules were inversions related. There exists the intramolecular N–H⋯O hydrogen bond of 2.610(3) Å from the 4-NH and the S(NO2). The dimers were linked into 1D chain by the pi–pi contact from the aryl moieties of 5,7-dinitropyrazolo[5,1-b]quinazolin-9(4H)-one with C–Cg = 3.228–3.398 Å to establish 1D chain in the b-axis (see lower part of the Figure). The chains were connected by the CH⋯O contact of 3.550 Å from the pyrazole CH and one O at the 7-NO2, and O–pi contact from the same O of the CH–O contact and the aryl kernel with O–Cg = 3.092 Å to get 2D sheet (Figure 2). The O–Cg separation was shorter than the document [9].

Here the respective 5,7-dinitropyrazolo[5,1-b]quinazolin-9(4H)-one at the adjacent chains were rotated by ca. 60° with each other. The sheets were stacked in the third direction by the N–H⋯O hydrogen bond of the N–H⋯C–O type with N–O = 2.807(3) Å, CH⋯O contact of 3.502 Å from the pyrazole CH and one O at the 5-NO2, CH⋯O contact of 3.067 Å from the same pyrazole CH and the C–O, CH⋯O contact of 3.138 Å from the phenyl CH and one O at the 5-NO2, CH⋯O contact of 3.104 Å from the phenyl CH and one O at the 5-NO2, and CH–N contact of 3.435 Å from the same phenyl CH and the pyrazole ring N to yield 3D ABAB layer net (see lower part of the Figure).

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