STUDY OF THE STRUCTURE OF 2,3-DIMETHYLQUINAZOLINE-4-ON

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Abstract: The non-H atoms of the title molecule, $C_{10}H_{10}N_2O$, are essentially coplanar, with a maximum deviation of 0.046 Å for the O atom. In the crystal, molecules are linked by weak C—H···O hydrogen bonds, forming chains along.
Key words: title molecule, structure, the title compound, displacement ellipsoids, 2-methylquinazoline-4-one, dimensional network

Introduction

Heterocyclic compounds are widely distributed in nature (drugs, alkaloids, pigments, and the others are included in the sentence of heterocyclic compounds), the magnitude of their importance in biological processes, in the reception of dyes and medicines, as well as the availability of the possibility of obtaining them from the waste products of Agriculture, from coal tar, which is the basis of the development of the Currently, two-thirds of the research conducted by chemist scientists around the world is aimed at the synthesis of heterocyclic compounds and the study of their properties. These compounds are easily formed from open-chain compounds and, as a result of the rupture of the ring, they again turn into open-chain compounds.

Method and results

The non-H atoms of the title molecule, $C_{10}H_{10}N_2O$, are essentially coplanar, with a maximum deviation of 0.046 (4) Å for the O atom. In the crystal, molecules are linked by weak C—H···O hydrogen bonds, forming chains along. In addition, weak C—H···π interactions and π–π stacking interactions between benzene and pyrimidine rings, with a centroid–centroid distance of 3.730 (3) Å, link the chains, forming a two-dimensional network parallel to (001).

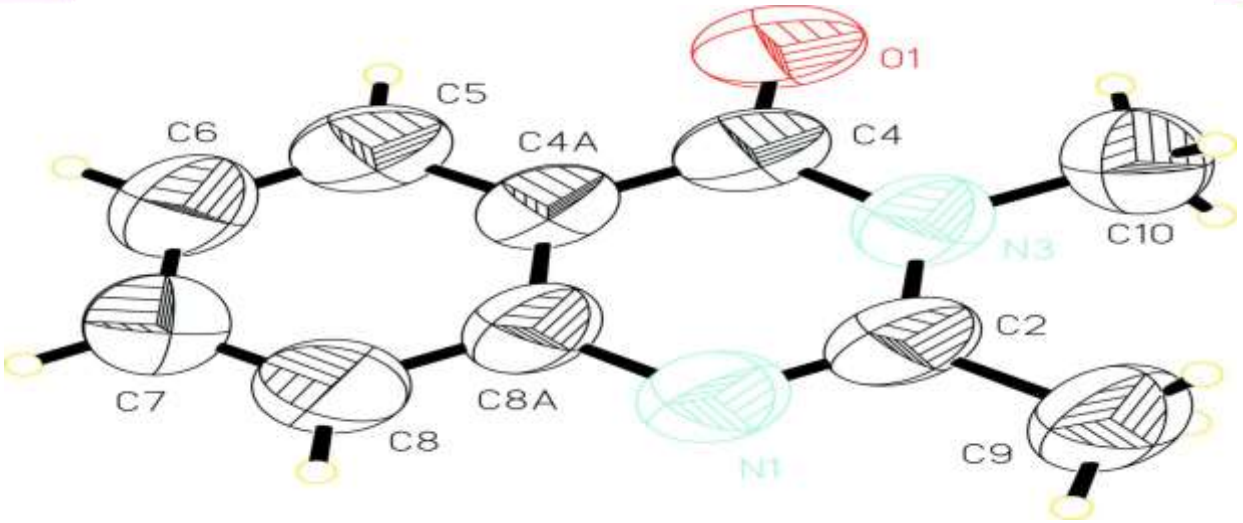


Figure 1. The molecular structure of the title compound with displacement ellipsoids are drawn at the 50% probability level.

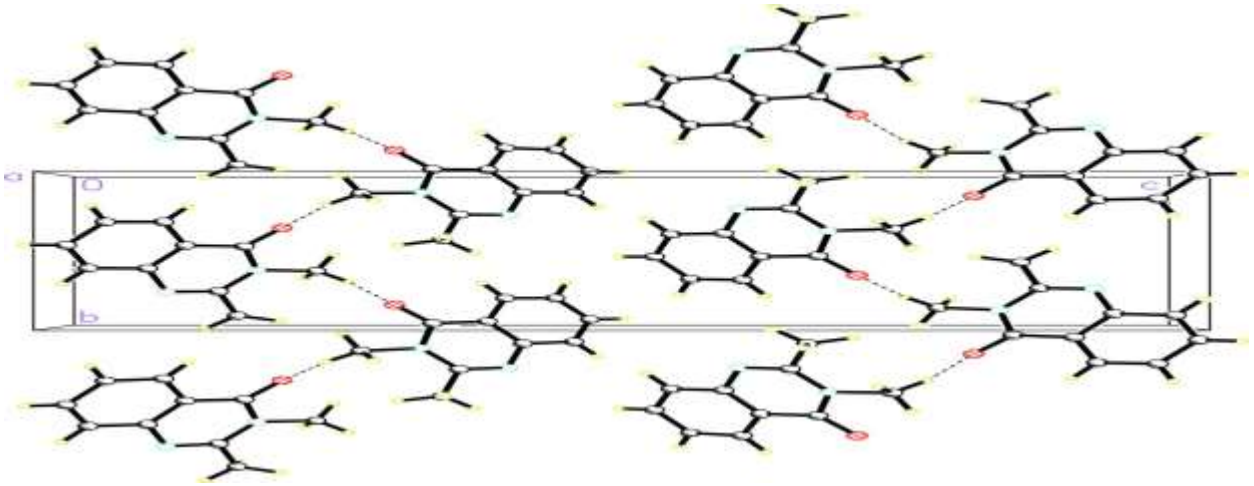
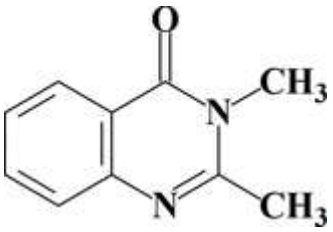


Figure 2. Crystal packing of the title compound showing a hydrogen bonds as dashed lines.



Experimental

- $C_{10}H_{10}N_2O$
- M_r = 174.20
- Orthorhombic, P 2_1 2_1 2_1
- a = 4.826 (2) Å
- b = 7.919 (3) Å
- c = 23.060 (8) Å
- V = 881.3 (11) Å^3

- Z = 4
- Cu Kα radiation
- μ = 0.71 mm^{-1}
- T = 293 K
- 0.40 × 0.10 × 0.08 mm
- Oxford Diffraction Xcalibur Ruby diffractometer
- Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2009) T_{min} = 0.041, T_{max} = 1.000
- 2236 measured reflections
- 1585 independent reflections
- 821 reflections with I > 2σ(I)
- R_{int} = 0.020
- R[F^2 > 2σ(F^2)] = 0.071
- wR(F^2) = 0.230
- S = 0.97
- 1585 reflections
- 121 parameters
- H-atom parameters constrained
- $\Delta\rho_{max}$ = 0.20 e $Å^{-3}$
- $\Delta\rho_{min}$ = −0.19 e $Å^{-3}$
- Absolute structure: Flack (1983), 507 Friedel pairs
- Absolute structure parameter: −0.3 (12)

Table 1

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the N1/C2/N3/C4/C4A/C8A ring.

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1^{i}	0.96	2.47	3.345 (8)	151
C10—H10B···Cg^{ii}	0.96	2.80	3.608 (6)	142

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) x-1, y, z.

The experimental part

10 mmoles of 2-methylquinazoline-4-ones are placed in a three-necked flask equipped with a drip funnel, a mechanical stirrer and a return refrigerator with a chlorocalcium tube. The substances are dissolved in 45 ml of absolute solvent and 2.5 mmol NaH is added with stirring. Stir for 30 minutes, and 1 mole of methyl iodide (dimethyl sulfate, methyltosylate) in 2 ml of solvent is also added

to the resulting sodium salt solution while stirring drop by drop. The reaction mixture is stirred at room temperature for 24 hours or heated in a boiling water bath for 3-4 hours. At the end of the reaction, the contents of the flask are treated with 150 ml of cold water, the resulting precipitate is filtered out. In cases where no precipitate falls out during decomposition, the reaction product is extracted three times with chloroform. Drying of the resulting product is carried out in a desiccator over anhydrous sodium or magnesium sulfate (Na_2SO_4, $MgSO_4$).

CONCLUSION

The non-H atoms are essentially co-planar, with a maximum deviation of 0.046 (4) Å for atom O1. In the crystal, molecules are linked by weak C—H···O hydrogen bonds to form chains along. In addition, weak C—H···π interactions and π–π stacking interactions between benzene and pyrimidine rings with a centroid–centroid distance of 3.730 (3)Å, link chains forming a two-dimensional network parallel. The bond distances and angles are in normal ranges.

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