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# The structure of 1-phenyl-3-benzoylamino-4-benzoylpyrazol-2-in-5-one

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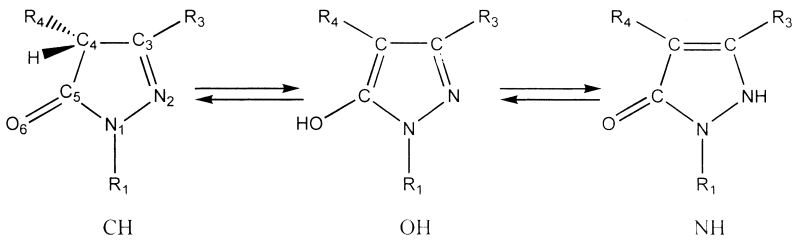
**Abstract**

Crystal and molecular structure of 1-phenyl-3-benzoylamino-4-benzoylpyrazol-2-in-5-one as a product of the benzoylation of 1-phenyl-3-benzoylaminopyrazol-2-in-5-one was characterised by X-ray single crystal diffraction. It is shown that 1-phenyl-3-benzoylamino-4-benzoylpyrazol-2-in-5-one exists in the solid phase in an NH-tautomeric form, which is stabilised by two intramolecular hydrogen bonds and one intermolecular bond with the solvate dioxane molecule, the latter being used as a solvent for recrystallisation. 

*Keywords*: Pyrazolones; Tautomerism; X-ray single crystal diffraction; Hydrogen bonding

## 1. Introduction

Pyrazol-5-ones are widely used as biologically active compounds, metal extractants, dyes, etc. [1–4]. They are structurally labile compounds capable to exist at least in three tautomeric forms:




The number of tautomeric forms may be increased upon introduction of labile substituents [5–7]. The tautomeric equilibrium depends not only on intrinsic properties of pyrazol-5-ones, but also on the influence of medium [1,7–9].

In the solid state, pyrazol-5-ones exist mainly in NH- or OH-forms [10–14], which are, as a rule, stabilised by intermolecular hydrogen bonding. The realisation of CH-forms is more rare [15], this

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