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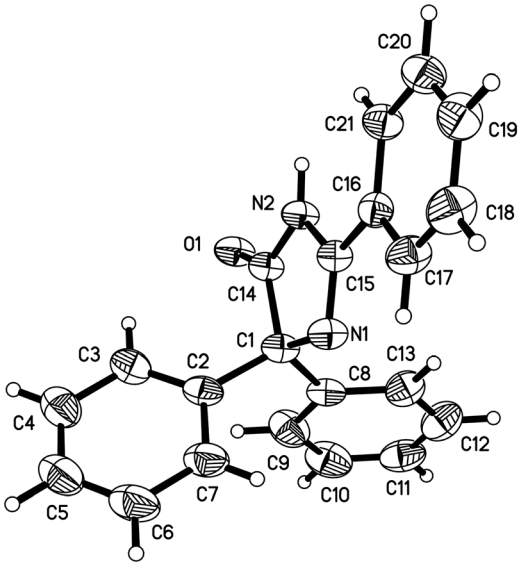
The crystal structure of 2,5,5-triphenyl-3,5-dihydro-4*H*-imidazol-4-one, $C_{21}H_{16}N_2O$



https://doi.org/10.1515/ncrs-2022-0082
Received February 19, 2022; accepted March 29, 2022; published online April 29, 2022

Abstract

$C_{21}H_{16}N_2O$, monoclinic, $P2_1/c$ (no. 14), a = 13.8987(3) Å, b = 15.0321(5) Å, c = 8.1727(2) Å, β = 99.337(2)°, V = 1684.87(8) Å^3, Z = 4, $R_{gt}(F)$ = 0.0411, $wR_{ref}(F^2)$ = 0.1137, T = 293(2) K.

CCDC no.: 2162862

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.22 × 0.15 × 0.11 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	0.61 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	72.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6667, 3234, 0.013
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2638
$N(param)_{refined}$:	217
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3, 4]

Source of material

The synthesis of the title compound was conducted in accord to reference [6] with slightly modification: In a 10 mL dried vessel, 36 mg NaOH (0.9 mmol) and 35.6 mg benzamidine hydrochloride hydrate (0.2 mmol) was purged with oxygen for three times, then 58.9 mg 1,2-diphenylethanone (0.3 mmol) and 0.8 mL pyridine was added. The vessel was sealed and heated at 353 K under stirring for 24 h. The volatiles were removed under vacuum and the residue was dissolved in absolute ethanol. Many colourless crystals were obtained, yield 75.6% (based on benzamidine hydrochloride hydrate).

Experimental details

The structure was solved by direct methods with the SHELXS-2018 program. All H-atoms from C and N atoms were positioned with idealised geometry and refined isotropic (U_{iso}(H) = 1.2U_{eq}(C) and 1.2U_{eq}(N)) using a riding model with C–H = 0.93 Å and N–H = 0.86 Å.

Comment

2-Heterocyclic-5,5-diphenylimidazolones are known as the potent human neuropeptide Y5 receptor antagonists and many analogues have been studied to obtained much better aqueous solubility and oral bioavailability [5]. Although the title compound has been studied earlier as one of the analogues in some places [5, 6], to the best of our knowledge, its single crystal structure has not been reported anywhere except a derivative 2-(anthracen-9-yl)-5,5-diphenyl-1,5-dihydro-4H-imidazol-4-one [7].

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.74319 (9)	0.51071 (10)	0.19701 (16)	0.0550 (3)
C2	0.79443 (9)	0.42408 (11)	0.25976 (17)	0.0585 (4)
C3	0.87390 (12)	0.42931 (14)	0.3870 (2)	0.0790 (5)
H3	0.894475	0.484378	0.431399	0.095*
C4	0.92251 (14)	0.35267 (17)	0.4478 (3)	0.0945 (6)
H4	0.976188	0.356759	0.531764	0.113*
C5	0.89227 (14)	0.27116 (16)	0.3855 (3)	0.0905 (6)
H5	0.924707	0.219982	0.427977	0.109*
C6	0.81470 (14)	0.26513 (14)	0.2614 (2)	0.0844 (5)
H6	0.794053	0.209650	0.219178	0.101*
C7	0.76597 (12)	0.34139 (12)	0.1972 (2)	0.0711 (4)
H7	0.713591	0.336517	0.111016	0.085*
C8	0.80142 (9)	0.56459 (11)	0.08791 (16)	0.0583 (4)
C9	0.85309 (13)	0.52248 (14)	−0.0210 (2)	0.0813 (5)
H9	0.856568	0.460703	−0.022206	0.098*
C10	0.89977 (14)	0.57185 (17)	−0.1285 (2)	0.0930 (6)
H10	0.934812	0.542920	−0.200477	0.112*
C11	0.89456 (12)	0.66279 (16)	−0.1294 (2)	0.0842 (5)
H11	0.925942	0.695599	−0.201527	0.101*
C12	0.84314 (14)	0.70495 (15)	−0.0238 (2)	0.0859 (5)
H12	0.839005	0.766706	−0.024803	0.103*
C13	0.79686 (12)	0.65631 (12)	0.0852 (2)	0.0714 (4)
H13	0.762391	0.685877	0.157170	0.086*
C14	0.64152 (9)	0.49473 (10)	0.09496 (16)	0.0531 (3)
C15	0.63067 (9)	0.56885 (9)	0.32955 (15)	0.0511 (3)
C16	0.57888 (10)	0.60890 (9)	0.45479 (16)	0.0519 (3)
C17	0.63227 (12)	0.63793 (12)	0.60360 (19)	0.0704 (4)
H17	0.699840	0.632665	0.622415	0.085*
C18	0.58522 (14)	0.67448 (13)	0.7232 (2)	0.0832 (5)
H18	0.621267	0.694001	0.822644	0.100*
C19	0.48535 (14)	0.68239 (12)	0.6971 (2)	0.0784 (5)
H19	0.454207	0.707566	0.778316	0.094*
C20	0.43147 (12)	0.65316 (12)	0.5510 (2)	0.0706 (4)
H20	0.363884	0.658192	0.533594	0.085*
C21	0.47804 (10)	0.61620 (10)	0.42975 (17)	0.0602 (3)
H21	0.441569	0.596173	0.331111	0.072*
N1	0.72346 (8)	0.56131 (9)	0.34261 (13)	0.0577 (3)
N2	0.57870 (7)	0.53273 (8)	0.18377 (13)	0.0536 (3)
H2	0.516390	0.534468	0.155187	0.064*
O1	0.62100 (7)	0.45767 (8)	−0.03928 (12)	0.0653 (3)

The title compound crystalizes as monoclinic, $P2_1/c$ (no. 14), with the formula $C_{21}H_{16}N_2O$. The title molecule consists of three phenyl groups and one imidazolone fragment. Two identical molecules are connected by two N2–H2···O1 hydrogen bonds to generate one dimer, which was reinforced by two weak C21–H21···O1 hydrogen bonds. All the bond lengths are similar to the reported results [6–11].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
Research funding: None declared.
Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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