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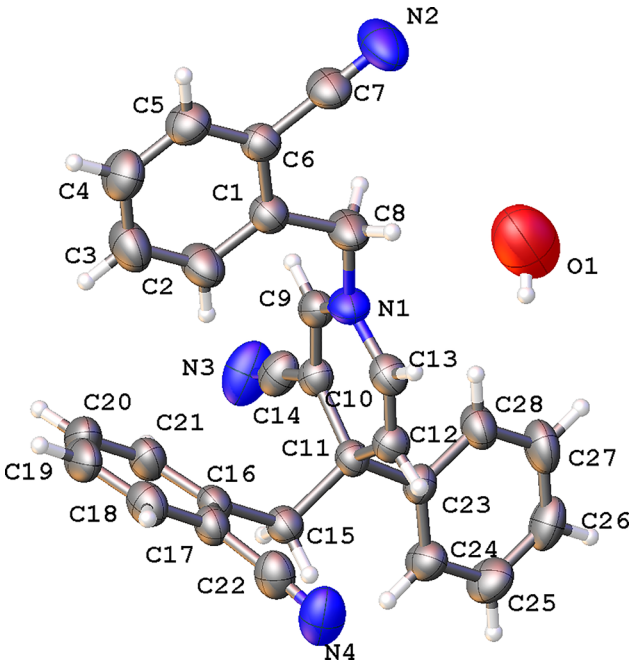
# Crystal structure of 1-(2-cyanobenzyl)-3-cyano-4-phenyl-4-(2-cyanobenzyl)-1,4-dihydropyridine monohydrate, $C_{56}H_{42}N_8O$

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**Abstract**

$C_{56}H_{42}N_8O$, orthorhombic, *Pbcn* (no. 60), $a$ = 17.885(3) Å, $b$ = 15.647(2) Å, $c$ = 16.189(2) Å, $V$ = 4530.4(11) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0464, $wR_{ref}(F^2)$ = 0.1219, T = 296.15 K.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.25 × 0.23 × 0.20 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 0.08 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 25.0°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 21952, 3990, 0.060 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs}$ > 2 σ($I_{obs}$), 2412 |
| $N(param)_{refined}$: | 295 |
| Programs: | Bruker [1], SHELX [2, 3] |

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.

## Source of material

API was obtained according to literature method [4, 5]. Mix 0.33 g (1.1 mmol) of the API and 0.21 g (1.1 mmol) of 2-(bromomethyl)benzonitrile in a 30 ml quartz tube, add 25 ml of methanol, and place it under a 410 nm LED light at room temperature for 24 h, evaporate and concentrate. The mixed solution of methanol and dichloromethane was recrystallized to obtain a white solid. This solid was dissolved in methanol: distilled water (10:1), and the solvent was slowly volatilized. After four days, a transparent block crystal was obtained.

## Experimental details

All hydrogen atoms were placed in the calculated positions.

## Comment

1,4–Dihydropyridine (1,4–DHP) is one of the most important heterocyclic moieties that possesses prominent therapeutic effects in a very versatile manner [5]. Photochemical reactions

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

| Atom | x | y | z | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.500000 | 0.8168 (2) | 0.750000 | 0.1525 (14) |
| H1 | 0.463300 | 0.854729 | 0.755550 | 0.229* |
| N1 | 0.31777 (9) | 0.63237 (12) | 0.72911 (10) | 0.0497 (5) |
| N2 | 0.57594 (13) | 0.61697 (17) | 0.61702 (13) | 0.0874 (7) |
| N3 | 0.14055 (14) | 0.42360 (13) | 0.81103 (12) | 0.0822 (7) |
| N4 | 0.11016 (13) | 0.88598 (14) | 0.70414 (13) | 0.0797 (7) |
| C1 | 0.38213 (12) | 0.61770 (13) | 0.59373 (12) | 0.0463 (5) |
| C2 | 0.31455 (13) | 0.61616 (15) | 0.55286 (13) | 0.0623 (7) |
| H2 | 0.270440 | 0.622313 | 0.582687 | 0.075* |
| C3 | 0.31139 (15) | 0.60558 (16) | 0.46806 (14) | 0.0709 (7) |
| H3 | 0.265235 | 0.604145 | 0.441638 | 0.085* |
| C4 | 0.37551 (16) | 0.59722 (16) | 0.42274 (14) | 0.0668 (7) |
| H4 | 0.372900 | 0.589821 | 0.365809 | 0.080* |
| C5 | 0.44331 (14) | 0.59976 (14) | 0.46130 (13) | 0.0583 (6) |
| H5 | 0.487033 | 0.594775 | 0.430572 | 0.070* |
| C6 | 0.44703 (12) | 0.60979 (12) | 0.54636 (12) | 0.0453 (5) |
| C7 | 0.51869 (14) | 0.61372 (15) | 0.58609 (13) | 0.0562 (6) |
| C8 | 0.38910 (12) | 0.62579 (16) | 0.68623 (13) | 0.0607 (7) |
| H8A | 0.415833 | 0.576412 | 0.707201 | 0.073* |
| H8B | 0.418731 | 0.676060 | 0.698793 | 0.073* |
| C9 | 0.27723 (12) | 0.56180 (14) | 0.74632 (11) | 0.0454 (5) |
| H9 | 0.295814 | 0.508998 | 0.729747 | 0.054* |
| C10 | 0.21147 (11) | 0.56403 (12) | 0.78613 (10) | 0.0394 (5) |
| C11 | 0.17427 (11) | 0.64614 (12) | 0.81647 (11) | 0.0375 (5) |
| C12 | 0.22774 (12) | 0.71841 (13) | 0.79783 (11) | 0.0422 (5) |
| H12 | 0.214498 | 0.772827 | 0.815715 | 0.051* |
| C13 | 0.29155 (12) | 0.71025 (14) | 0.75825 (11) | 0.0457 (5) |
| H13 | 0.320416 | 0.758829 | 0.749388 | 0.055* |
| C14 | 0.17361 (13) | 0.48575 (14) | 0.80034 (12) | 0.0521 (6) |
| C15 | 0.09818 (11) | 0.66033 (13) | 0.77198 (11) | 0.0432 (5) |
| H15A | 0.064173 | 0.615032 | 0.788164 | 0.052* |
| H15B | 0.076998 | 0.713945 | 0.790872 | 0.052* |
| C16 | 0.10285 (10) | 0.66226 (13) | 0.67900 (11) | 0.0411 (5) |
| C17 | 0.11115 (11) | 0.73801 (13) | 0.63458 (12) | 0.0449 (5) |
| C18 | 0.11678 (12) | 0.73838 (16) | 0.54851 (12) | 0.0557 (6) |
| H18 | 0.123218 | 0.789690 | 0.520392 | 0.067* |
| C19 | 0.11282 (13) | 0.66308 (17) | 0.50559 (13) | 0.0607 (7) |
| H19 | 0.116516 | 0.663037 | 0.448292 | 0.073* |
| C20 | 0.10338 (13) | 0.58773 (16) | 0.54764 (14) | 0.0629 (7) |
| H20 | 0.100138 | 0.536547 | 0.518664 | 0.075* |
| C21 | 0.09866 (12) | 0.58752 (14) | 0.63254 (13) | 0.0537 (6) |
| H21 | 0.092475 | 0.535676 | 0.659785 | 0.064* |
| C22 | 0.11166 (13) | 0.81935 (16) | 0.67503 (13) | 0.0563 (6) |
| C23 | 0.16366 (11) | 0.64138 (12) | 0.91121 (11) | 0.0398 (5) |
| C24 | 0.09794 (13) | 0.66114 (14) | 0.95156 (12) | 0.0526 (6) |
| H24 | 0.056233 | 0.677137 | 0.920935 | 0.063* |
| C25 | 0.09299 (14) | 0.65756 (15) | 1.03701 (13) | 0.0627 (7) |
| H25 | 0.048250 | 0.671418 | 1.063056 | 0.075* |
| C26 | 0.15338 (16) | 0.63384 (14) | 1.08298 (13) | 0.0607 (7) |
| H26 | 0.149931 | 0.631342 | 1.140246 | 0.073* |
| C27 | 0.21919 (15) | 0.61370 (15) | 1.04429 (13) | 0.0641 (7) |
| H27 | 0.260481 | 0.597430 | 1.075455 | 0.077* |
| C28 | 0.22456 (13) | 0.61743 (14) | 0.95908 (12) | 0.0551 (6) |
| H28 | 0.269572 | 0.603716 | 0.933551 | 0.066* |

have been widely used in various synthetic reactions [6, 7]. In particular, six-membered rings with symmetrical double bond structure are often used as educts for photoreactions. Earlier, 3–cyanopyridine, benzyl bromide or methyl bromide and phenylmagnesium bromide were used as educts to form 1-(2-cyanobenzyl)-3-cyano-4-phenyl-1,4-dihydropyridine [4]. This time, 2-(bromomethyl)benzonitrile and 1-(2-cyanobenzyl)-3-cyano-4-phenyl-1,4-dihydropyridine were used and different photoreaction solvents were used to obtain a new compound through light irradiation.

The asymmetric unit is composed of a molecule of 1-(2-cyanobenzyl)-3-cyano-4-phenyl-4-(2-cyanobenzyl)-1,4-dihydropyridine and a molecule of crystalline water.

In the molecules forming the title crystal structure all rings are significantly inclined to one another (see the Figure). The bond lengths and angles are in the expected ranges [8].

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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