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The crystal structure of 3-methoxyphenanthridin-6(5H)-one, C_{14}H_{11}NO_{2}

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Abstract
C_{14}H_{11}NO_{2}, monoclinic, P2_{1}/c (no. 14), a = 12.7731(19) Å, b = 5.4767(9) Å, c = 17.3616(18) Å, \( \beta = 119.747(7)^{\circ} \), V = 1054.5(3) Å\(^3\), Z = 4, \( R_{gt}(F) = 0.0562, wR_{ref}(F^2) = 0.1907, T = 298(2) \) K.

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The molecular structure of the title crystal structure is shown in the figure (atoms are drawn with arbitrary radii). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material
The title compound was obtained according to the literature method [5]. Single crystal suitable for X-ray diffraction were grown during slow evaporation of a mixture of ethyl acetate and petroleum ether.

Experimental details
H atoms bonded were positioned geometrically and refined using a riding model, with C—H = 0.93/0.96/0.97 Å and N—H = 0.86 Å with \( U_{iso} = 1.2 \) times \( U_{eq}(C) \) and 1.2 times \( U_{eq}(N) \).

Discussion
In recent years, phenanthridinone has been found to be a key core unit in some natural products with important biological...
activities [6–8] and drug molecules for the treatment of nerve diseases [9–11]. Thus, the synthesis and crystal structures of various phenanthridinone derivatives have attracted great attention [5, 12].

There is one molecule in the asymmetric unit. In the title compound, the two benzo rings and the pyridin-2(1H)-one ring are in the same plane, indicating the compound is an almost planar molecule. This planar parent structure is also present in the previously reported phenanthridinone derivatives [5, 13]. The molecules of the title compound in the same layer are connected by N(1)—H(1)⋯O(1) hydrogen bonds (donor-acceptor distance: 2.829 Å), which is in agreement with that in previously reported structure of phenanthridone [13]. The molecules in the next layers are stabilized by two kinds of aromatic C—H⋯π (2.805 and 3.441 Å) and π⋯π stacking interaction with a distance of 3.686 Å between the pyridin-2(1H)-one moieties.

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References