Ahmed M. El-Agrody, Abd El-Galil E. Amr*, Nermien M. Sabry, Mohamed A. Al-Omar and Hazem A. Ghabbour

Crystal structure of 3-amino-9-methoxy-1-phenyl-1H-benzo[f]chromene-2-carbonitrile, C_{21}H_{16}N_{2}O_{2}

Abstract

C_{21}H_{16}N_{2}O_{2}, monoclinic, P2_1/n (no. 14), a = 13.4768(7) Å, b = 6.9225(3) Å, c = 18.2840(8) Å, \( \beta = 107.601(2) \)°, \( V = 1625.92(13) \) Å\(^3\), \( Z = 4 \), \( R_{	ext{gt}}(F) = 0.0593 \), \( wR_{	ext{gt}}(F^2) = 0.1529 \), \( T = 100 \) K.

CCDC no.: 1474776

The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

| Crystal: Colourless blocks |
| Wavelength: Mo Kα radiation (0.71073 Å) |
| μ: 0.9 cm\(^{-1}\) |
| Diffractometer, scan mode: Bruker APEX-II, φ and ω |
| 2θ_{max}, completeness: 54°, >99% |
| N(hkl)_{measured}, N(hkl)_{unique}, R_{int}: 20809, 3545, 0.082 |
| Criterion for I_{obs}, N(hkl)_{gt}: \( I_{obs} > 2 \delta(I_{obs}) \), 2057 |
| N(param)_{refined}: 235 |
| Programs: SHELX [20], Bruker programs [21] |

Source of material

A mixture of 7-methoxy-2-naphthol (0.01 mol), malononitrile (0.01 mol), benzaldehyde (0.01 mol), ethanol (30 mL) and piperidine (0.5 mL) was heated under reflux for 1 h. After complete precipitation occurred the solid product was collected by filtration, washed by methanol and recrystallized from ethanol to give the title compound as colourless crystals; yield 89%; M.p.: 528–529 K.

Experimental details

Carbon-bound hydrogen atoms were placed in calculated positions and were included in the refinement in the riding model approximation. The H atoms of the methyl groups were allowed to rotate with a fixed angle around the C–C bond to best fit the experimental electron density.
isotropic displacement parameters (Å²), estrogenic anticoagulant and antispasmolytic [14],

Discussion

Chromene and benzochromene derivatives have attracted considerable interest owing to their biological and pharmaceutical activities such as antibacterial [1–3], antifungal [4–6], vascular-disrupting [7], antioxidant [8, 9], anticancer [10–13], estrogenic anticoagulant and antispasmodic [14], antileishmanial [15], antiproliferative and apoptosis inducing [16–19].

In the title structure the asymmetric unit contains one independent molecule. All bond lengths and angles are in the expected ranges. The phenyl ring (C16–C20) is perpendicular to the plane of the rest of the molecule (∠).

The molecules are connected in the crystal structure via two symmetry related strong classical intermolecular hydrogen bonds, N1—H2N1 ⋯ N2 (H⋯A distance = 2.20(3) Å; \(N—H⋯N\) angle = 162(3)°; symmetry code: (i) \(-x + 1, -y + 1, -z + 2\).

Acknowledgements: The project was financially supported by King Saud University, Vice Deanship of Research Chairs.

References


