Crystal structure of 5,6,3′,4′,5′-pentamethoxy-flavone dihydrate, C_{20}H_{24}O_{9}

Abstract

C_{20}H_{24}O_{9}, monoclinic, P2_1/c (no. 14), \( a = 9.7647(2) \) Å, \( b = 7.3098(10) \) Å, \( c = 27.7075(4) \) Å, \( \beta = 92.138(10) \)°, \( V = 1976.33(6) \) Å³, \( Z = 4, R_{gt}(F) = 0.0479, wR_{ref}(F^2) = 0.1504, T = 300(2) \) K.

Table 1: Data collection and handling.

| Crystal: | Colourless block |
| Size: | 0.37 x 0.33 x 0.19 mm |
| Wavelength: | Mo Kα radiation (0.71073 Å) |
| μ: | 0.11 mm⁻¹ |
| Diffractometer, scan mode: | Bruker APEX-II, ϕ and ω |
| θ_{max}, completeness: | 28.3°, >99 % |
| N(hkl)measured-N(hkl)unique, R_{int}: | 66,870, 4907, 0.050 |
| Criterion for I_{obs}, N(hkl): | I_{obs} > 2 σ(I_{obs}), 3715 |
| N(param)_refined: | 278 |
| Programs: | Olex2,¹ SHELX,² Bruker,³ Mercury⁴ |

The ORTEP diagram drawn at 50 % probability ellipsoid is shown in figure. Table 1 contains the crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

The title compound is derived from the plants of Knema malayana Warb. The product (5.23 g) was separated and purified from the crude product by silica gel column chromatography. Colorless crystals were obtained after chloroform-methanol recrystallization for 3 days. The systematic name is 5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-1-benzopyran-4-one hydrate.
2 Experimental details

The hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

Flavonoids are a group of compounds that are found in many plants. They are an important group of natural products that can be recognised by their 2-phenylchromone core structure. This category encompasses various subclasses, including flavones, isoflavones, flavonols, anthocyanidins, flavanones, flavanols, chalcones, and aurones. Recent advancements in pharmacological research underscore the multifaceted biological activities exhibited by flavonoids, ranging from potent antioxidant, anti-inflammatory properties to cytotoxic effects, and antimicrobial and antiviral activities.

The title compound includes five methoxy substituents. Examination of the crystal structure reveals bond lengths and angles consistent with established norms. The key lengths and angles obtained from the title structure are within the normal range and are consistent with those previously reported in similar structures. Notably, the ketone bond (C19-O3) is observed at a distance of 1.3563(16) Å, while the methoxy substituents exhibit bond lengths of 1.428(2) Å (C19-O3), 1.431(3) Å (C26-O3), 1.431(3) Å (C20-O1), 1.431(3) Å (C17-O2) and 1.415(3) Å (C16-O3).

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References