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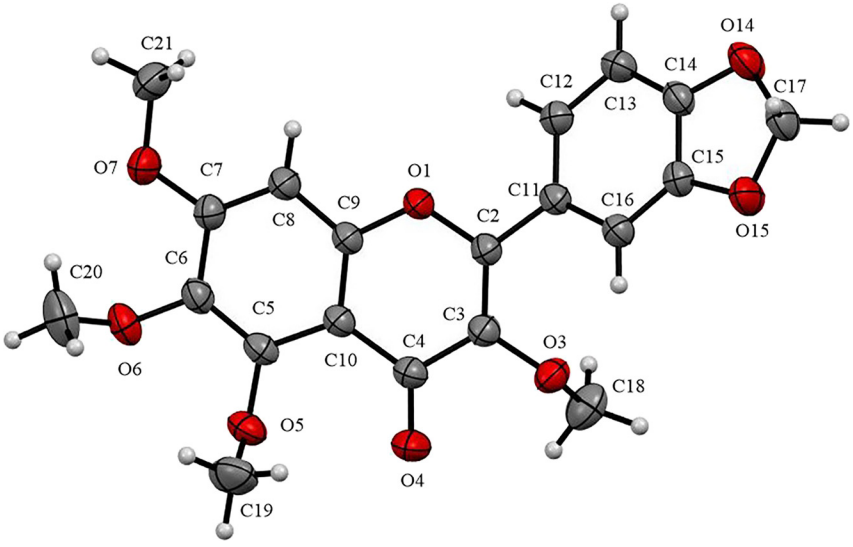
Crystal structure of 3,5,6,7-tetramethoxy-3′,4′-methylenedioxy-flavone, $C_{20}H_{18}O_8$



https://doi.org/10.1515/ncrs-2022-0337
Received June 29, 2022; accepted August 19, 2022;
published online September 2, 2022

Abstract

$C_{20}H_{18}O_8$, monoclinic, $P2_1/c$ (no. 14), a = 7.3855(2) Å, b = 28.1424(9) Å, c = 8.5863(3) Å, β = 98.4040(10)°, V = 1765.46(10) Å^3, Z = 4, $R_{gt}(F)$ = 0.0545, $wR_{ref}(F^2)$ = 0.1641, T = 273(2) K.

CCDC no.: 2202403

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:	Yellow raphides
Size:	0.17 × 0.19 × 0.22 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.11 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	35.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	39241, 7728, 0.032
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5424
$N(param)_{refined}$:	257
Programs:	Olex2 [1], Bruker [2], SHELX [3], Diamond [4]

Source of material

The title compound is derived from the plants of *Heracleum*. The crude product (4.125 g) was separated from the mixed filtrate by silica gel column chromatography. Then, the yellow solution was further separated and purified from the crude product by silica gel column chromatography. After one day of slow evaporation, a yellow needle crystal suitable for X-ray diffraction was obtained. The systematic name is 2-(benzo[*d*][1,3]dioxol-5-yl)-3,5,6,7-tetramethoxy-4H-chromen-4-one.

Experimental details

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

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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}
O1	0.41974 (14)	0.93416 (3)	0.84250 (12)	0.0501 (2)
O2	0.26736 (11)	0.73239 (3)	0.65682 (11)	0.03883 (18)
O3	0.32561 (14)	0.53802 (3)	0.67363 (11)	0.0466 (2)
O4	0.17936 (15)	0.95173 (3)	0.64706 (12)	0.0506 (2)
O5	0.62007 (12)	0.58948 (3)	0.79274 (11)	0.0443 (2)
O6	0.00949 (13)	0.57995 (3)	0.55171 (13)	0.0504 (2)
O7	0.76812 (13)	0.68061 (3)	0.83871 (14)	0.0564 (3)
O8	0.71194 (11)	0.77660 (3)	0.82714 (11)	0.04057 (19)
C1	0.2864 (2)	0.96943 (4)	0.78820 (17)	0.0492 (3)
H3	0.346242	0.998887	0.766601	0.059*
H1	0.208513	0.975524	0.867676	0.059*
C2	0.35994 (15)	0.89346 (4)	0.76363 (13)	0.0348 (2)
C3	0.42856 (15)	0.84846 (4)	0.78895 (13)	0.0353 (2)
H18	0.523734	0.841891	0.869543	0.042*
C4	0.34795 (14)	0.81250 (3)	0.68689 (12)	0.03203 (19)
C5	0.40735 (14)	0.76271 (4)	0.70915 (13)	0.03264 (19)
C6	0.29210 (14)	0.68434 (3)	0.66615 (13)	0.0334 (2)
C7	0.13726 (15)	0.65835 (4)	0.60661 (14)	0.0372 (2)
H12	0.028980	0.673611	0.565774	0.045*
C8	0.14798 (16)	0.60937 (4)	0.60950 (14)	0.0370 (2)
C9	0.31191 (16)	0.58662 (4)	0.67604 (13)	0.0367 (2)
C10	0.2176 (3)	0.51330 (6)	0.7719 (2)	0.0705 (5)
H2	0.252227	0.523142	0.879151	0.106*
H13	0.237129	0.479725	0.763591	0.106*
H14	0.090547	0.520364	0.739140	0.106*
C11	0.21760 (16)	0.90404 (4)	0.64477 (13)	0.0365 (2)
C12	0.13877 (17)	0.86993 (4)	0.54288 (14)	0.0406 (2)
H4	0.044708	0.877204	0.462077	0.049*
C13	0.20635 (15)	0.82370 (4)	0.56607 (13)	0.0368 (2)
H5	0.155588	0.799687	0.499117	0.044*
C14	0.45796 (14)	0.66372 (4)	0.73027 (12)	0.03304 (19)
C15	0.46310 (15)	0.61321 (4)	0.73530 (12)	0.0346 (2)
C16	0.6503 (2)	0.58457 (7)	0.95914 (19)	0.0641 (4)
H8	0.656785	0.615466	1.007010	0.096*
H7	0.763200	0.567952	0.990671	0.096*
H6	0.551239	0.566968	0.992212	0.096*
C17	−0.16038 (19)	0.60096 (5)	0.4882 (2)	0.0544 (3)
H11	−0.196791	0.623189	0.562593	0.082*
H9	−0.251823	0.576646	0.466956	0.082*
H10	−0.147239	0.617235	0.392255	0.082*
C18	0.61386 (15)	0.69478 (4)	0.78574 (13)	0.0364 (2)
C19	0.57435 (14)	0.74568 (4)	0.77193 (13)	0.0343 (2)
C20	0.8564 (2)	0.77880 (6)	0.7330 (2)	0.0571 (4)
H16	0.929498	0.750535	0.749100	0.086*
H15	0.931488	0.806085	0.762880	0.086*
H17	0.805041	0.781249	0.623973	0.086*

Comment

Flavonoids are widely distributed in nature and play an important role in natural phenolic compounds. Modern pharmacological research shows that flavonoids have strong biological activities in anti-inflammatory, antibacterial, anti-cancer, anti-virus, nerve protection, anti-oxidation and so on [5–10]. Therefore, it is of great significance to further study and clarify the structure of flavonoids.

The title compound contains a chromene moiety with four methoxy groups and the benzo[*d*][1,3]dioxol-5-yl moiety at the 2-position of the chromene (see the figure). The bond lengths and angles which were derived from the title structure are within normal ranges [11]: keto group shows a C=O distance of 1.2298(13) Å (C_{18}—O_7); the C—O bonds in methoxy groups are 1.4245(19) Å (C_{10}—O_3), 1.4202(18) Å (C_{16}—O_5), 1.4216(17) Å (C_{17}—O_6), 1.4305(17) (17) Å (C_{20}—O_8).

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This work was funded by special project of scientific research innovation and exploration of Guizhou University of traditional Chinese medicine in 2021 [No. 2019YFC171250303].

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

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