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Flavocommelin Octaacetate

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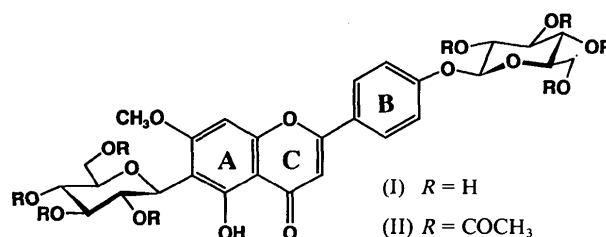
Abstract

Flavocommelin, 6- β -D-glucopyranosyl-2-[4-(β -D-glucopyranosyloxy)phenyl]-5-hydroxy-7-methoxy-4H-1-benzopyran-4-one, is a flavonoid component of a blue pigment, commelin, which is isolated from the petals of *Commelina communis*. The crystal structure of the octaacetate derivative, 5-hydroxy-7-methoxy-6-(3,4,5,6-tetra-O-acetyl- β -D-glucopyranosyl)-2-[4-(3,4,5,6-tetra-O-acetyl- β -D-glucopyranosyloxy)-phenyl]-4H-1-benzopyran-4-one, $C_{44}H_{48}O_{23}$, has been determined by X-ray diffraction. In the crystal, the molecules are arranged parallel to each other according to the periodicity of the crystal lattice. However, intermolecular stacking of the flavanone skeletons is not observed. This suggests that the

hydrophilicity of the glucose moieties is one of the important factors governing the self association.

Comment

The mechanism of the color variation and stabilization of anthocyanins has been investigated previously (Goto & Kondo, 1991). The crystal structure of commelin has been determined and revealed that the pigment is a metal-complex anthocyanin (Kondo *et al.*, 1992). In the pigment there exists hydrophobic stacking of the aromatic rings of the anthocyanin and flavone molecules. One of the components, flavocommelin (I), also shows self association in condensed aqueous solutions (Goto, Yoshida, Yoshikane & Kondo, 1990). Because the crystallization of (I) is difficult, the acetate derivative, (II), was prepared.



There are many reports of crystal structures of flavone compounds, but none of them have a sugar moiety except aciculatin (Krause & Eggleston, 1991). In the crystal of aciculatin (monoclinic, space group $I2_1$, $Z = 8$), the aromatic rings are stacked: two independent flavone molecules lie separately on 2₁ screw axes with the flavanone skeletons almost perpendicular to the screw axes. The cell parameter b [7.371 (2) Å] is, therefore, roughly four times the van der Waals radius of the aromatic C atom (1.77 Å).

The molecular structure of the title compound is shown in Fig. 1. The C22–C23–C25–O4 plane of the hexopyranosyl ring of the glucose moiety connected by the O–glucopyranosyloxy bond is inclined at 30.1 (3)° to the phenyl ring *B*, while the C17–C18–C20–O3 plane of the other glucopyranosyl connected by the C–glucopyranosyl bond is almost perpendicular to the benzene ring *A* [84.4 (2)°], as a result of steric interactions. The phenyl ring *B* not only rotates around the C1–C10 bond but is also slightly bent with respect to the pyran plane, *C*. This bending is measured by the shift, S , of the center of ring *B* from the plane of ring *C* [$S = 0.25$ (2) Å]. Similar bending is also observed in other flavone crystals, as shown in Table 3. The *A*, *B* and *C* rings are essentially planar. The bending between the *B* and *C* rings must be a result of the crystal packing. Six of the 18 flavone molecules, whose deformations were calculated based on the crystal structure data, have S

values of less than 0.06 Å. The benzopyran moieties are not completely planar and the dihedral angles between the *A* and *C* rings are in the range 0.3 (1)–4.4 (4)°.

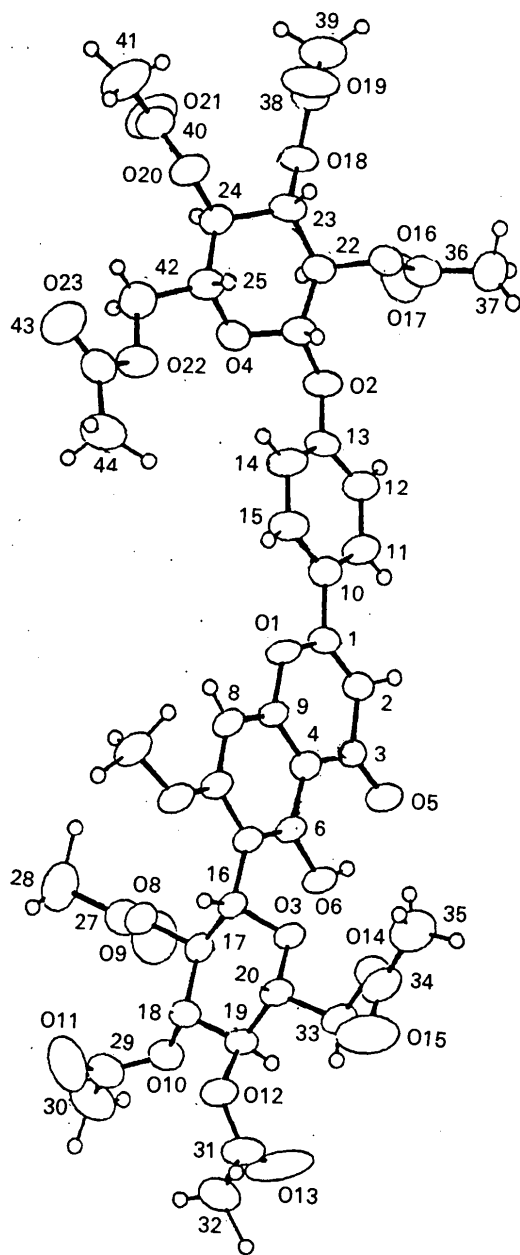


Fig. 1. Molecular structure with the atom-numbering scheme; the C atoms are labeled with numbers only.

Experimental

The compound was isolated from *Commelina communis*. A solution of flavocommelin (500 mg) in Ac₂O (4 ml)/pyridine (6 ml) was allowed to stand at room temperature for 24 h and then worked up as usual to give an oil which was purified by

preparative TLC using CHCl₃/AcOEt (1:1) to afford a colorless oil of acetylflavocommelin (480 mg). The crystals were grown from AcOEt, benzene and acetone mixture.

Crystal data

C₄₄H₄₈O₂₃
M_r = 944.85
 Triclinic
*P*1
a = 10.299 (4) Å
b = 20.221 (5) Å
c = 5.696 (5) Å
 α = 93.01 (4)°
 β = 94.46 (6)°
 γ = 81.12 (3)°
V = 1167 (1) Å³
Z = 1

D_x = 1.34 Mg m⁻³
 Synchrotron radiation
 λ = 1.0000 Å
 Cell parameters from 25 reflections
 θ = 5–11° (Mo *K*α)
 μ = 0.248 mm⁻¹ (λ = 1 Å)
T = 288 K
 Needle
 0.45 × 0.12 × 0.07 mm
 Pale yellow

Data collection

Weissenberg camera diffractometer
 Imaging plates
 Absorption correction: none
 3838 measured reflections
 3838 independent reflections

3823 observed reflections
 $[|F_o| > 3\sigma(|F_o|)]$
 θ_{\max} = 41.9°
 h = -8 → 15
 k = -30 → 20
 l = -3 → 3

Refinement

Refinement on *F*
R = 0.071
wR = 0.069
S = 1.16
 3823 reflections
 745 parameters
 Only coordinates of H atoms refined
 $w = 1/[\sigma^2(|F_o|) + (0.015|F_o|)^2]^{1/2}$

$(\Delta/\sigma)_{\max}$ = 0.15
 $\Delta\rho_{\max}$ = 0.22 e Å⁻³
 $\Delta\rho_{\min}$ = -0.26 e Å⁻³
 Extinction correction: none
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$B_{eq} = (8\pi^2/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j.$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B_{eq}</i>
O1†	0.80813	0.84716	0.65031	4.0 (1)
O2	0.4108 (4)	1.0715 (2)	0.137 (1)	4.1 (1)
O3	1.2852 (4)	0.6416 (2)	1.071 (1)	3.4 (1)
O4	0.2257 (4)	1.0505 (2)	0.300 (1)	4.0 (1)
O5	1.1544 (4)	0.7940 (3)	0.338 (1)	4.7 (1)
O6	1.2108 (4)	0.6937 (3)	0.614 (1)	4.1 (1)
O7	0.9199 (4)	0.6746 (3)	1.195 (1)	4.5 (1)
O8	1.0385 (4)	0.5439 (2)	0.808 (1)	3.9 (2)
O9	1.0632 (8)	0.5274 (4)	0.416 (2)	7.2 (2)
O10	1.2879 (4)	0.4541 (2)	0.778 (1)	4.4 (1)
O11	1.1757 (9)	0.3826 (3)	0.932 (2)	8.8 (3)
O12	1.4455 (4)	0.4749 (2)	1.232 (1)	4.6 (1)
O13	1.6308 (7)	0.4536 (4)	1.053 (2)	10.3 (3)
O14	1.4731 (4)	0.6802 (2)	1.402 (1)	4.5 (2)
O15	1.5830 (6)	0.6374 (4)	1.723 (1)	7.9 (2)
O16	0.3112 (4)	1.2098 (2)	0.154 (1)	3.8 (2)
O17	0.3358 (7)	1.1960 (4)	-0.234 (2)	6.5 (2)
O18	0.0297 (4)	1.2275 (2)	0.080 (1)	4.1 (1)
O19	-0.0557 (6)	1.3028 (3)	0.348 (2)	7.2 (2)
O20	-0.0769 (4)	1.1534 (3)	0.464 (1)	4.7 (1)
O21	-0.2307 (6)	1.1603 (4)	0.156 (2)	7.6 (3)
O22	0.1557 (5)	0.9736 (3)	0.641 (1)	5.8 (2)

O23	0.0139 (6)	0.9605 (4)	0.901 (1)	6.9 (2)	C5—C6—C7	117.8 (5)	C13—C14—C15	119.1 (7)
C1	0.8348 (5)	0.8793 (3)	0.461 (1)	3.6 (2)	C5—C6—C16	123.6 (5)	C14—C15—C10	121.4 (9)
C2	0.9476 (5)	0.8634 (3)	0.351 (2)	3.8 (2)	C7—C6—C16	118.6 (6)		
C3	1.0480 (5)	0.8088 (3)	0.436 (1)	3.5 (2)				
C4	1.0158 (5)	0.7735 (3)	0.627 (1)	3.2 (2)				
C5	1.0989 (5)	0.7164 (3)	0.721 (1)	3.1 (2)				
C6	1.0674 (5)	0.6840 (3)	0.909 (1)	3.2 (2)				
C7	0.9446 (5)	0.7077 (3)	1.007 (1)	3.3 (2)				
C8	0.8580 (5)	0.7613 (3)	0.917 (2)	3.7 (2)				
C9	0.8963 (5)	0.7939 (3)	0.734 (1)	3.4 (2)				
C10	0.7242 (5)	0.9312 (3)	0.384 (1)	3.8 (2)				
C11	0.7285 (6)	0.9669 (4)	0.186 (2)	4.8 (2)				
C12	0.6238 (6)	1.0142 (3)	0.110 (2)	4.7 (2)				
C13	0.5109 (5)	1.0254 (3)	0.235 (2)	3.6 (2)				
C14	0.5045 (6)	0.9915 (4)	0.436 (2)	4.8 (2)				
C15	0.6109 (6)	0.9445 (4)	0.510 (2)	4.8 (2)				
C16	1.1555 (5)	0.6249 (3)	1.017 (1)	3.0 (2)				
C17	1.1677 (5)	0.5630 (3)	0.849 (1)	3.2 (2)				
C18	1.2589 (5)	0.5050 (3)	0.966 (2)	3.5 (2)				
C19	1.3864 (5)	0.5249 (3)	1.066 (1)	3.2 (2)				
C20	1.3644 (5)	0.5923 (3)	1.210 (1)	3.2 (2)				
C21	0.3080 (6)	1.0994 (3)	0.283 (2)	3.8 (2)				
C22	0.2313 (6)	1.1573 (3)	0.144 (2)	3.6 (2)				
C23	0.1028 (6)	1.1857 (3)	0.257 (2)	3.5 (2)				
C24	0.0269 (5)	1.1292 (3)	0.309 (2)	3.5 (2)				
C25	0.1206 (6)	1.0760 (3)	0.449 (2)	3.7 (2)				
C26	0.7896 (6)	0.6854 (4)	1.272 (2)	5.3 (3)				
C27	1.0004 (7)	0.5268 (4)	0.585 (2)	4.2 (3)				
C28	0.8646 (8)	0.5062 (6)	0.577 (2)	7.8 (4)				
C29	1.2297 (6)	0.3986 (4)	0.772 (2)	5.0 (2)				
C30	1.244 (1)	0.3603 (4)	0.546 (2)	6.8 (4)				
C31	1.5685 (7)	0.4438 (3)	1.207 (2)	5.1 (2)				
C32	1.6161 (8)	0.3995 (4)	1.404 (2)	6.6 (3)				
C33	1.4944 (6)	0.6168 (3)	1.270 (2)	3.9 (2)				
C34	1.5189 (6)	0.6830 (4)	1.625 (2)	5.0 (3)				
C35	1.4830 (9)	0.7512 (5)	1.737 (3)	7.7 (4)				
C36	0.3656 (7)	1.2212 (3)	-0.045 (2)	4.4 (3)				
C37	0.4630 (8)	1.2691 (4)	0.004 (2)	5.9 (3)				
C38	-0.0455 (6)	1.2854 (3)	0.148 (2)	4.8 (3)				
C39	-0.1090 (8)	1.3219 (5)	-0.063 (2)	6.2 (3)				
C40	-0.2032 (6)	1.1641 (4)	0.362 (2)	5.6 (3)				
C41	-0.2980 (9)	1.1820 (6)	0.546 (3)	8.4 (4)				
C42	0.0560 (7)	1.0181 (4)	0.507 (2)	5.6 (3)				
C43	0.1234 (7)	0.9488 (3)	0.834 (2)	5.0 (2)				
C44	0.2374 (9)	0.9042 (4)	0.951 (2)	6.7 (3)				
HO6	1.219 (8)	0.717 (5)	0.49 (2)	5.00				

† Atom fixed.

Table 2. Selected geometric parameters (Å, °)

O1—C1	1.357 (8)	C5—C6	1.37 (1)
O1—C9	1.376 (5)	C6—C7	1.427 (8)
O2—C13	1.382 (7)	C6—C16	1.514 (8)
O2—C21	1.426 (9)	C7—C8	1.386 (8)
O5—C3	1.257 (8)	C8—C9	1.38 (1)
O6—C5	1.352 (8)	C10—C11	1.38 (1)
C1—C2	1.347 (9)	C10—C15	1.40 (1)
C1—C10	1.480 (8)	C11—C12	1.385 (9)
C2—C3	1.466 (8)	C12—C13	1.39 (1)
C3—C4	1.42 (1)	C13—C14	1.38 (1)
C4—C9	1.410 (8)	C14—C15	1.388 (9)
C4—C5	1.427 (8)		
C1—O1—C9	119.9 (4)	O7—C7—C8	122.8 (6)
C13—O2—C21	117.5 (7)	O7—C7—C6	115.2 (5)
C2—C1—O1	123.2 (5)	C8—C7—C6	122.0 (7)
C2—C1—C10	124.6 (7)	C9—C8—C7	118.0 (6)
O1—C1—C10	112.2 (5)	O1—C9—C8	116.2 (4)
C1—C2—C3	119.9 (7)	O1—C9—C4	120.5 (6)
O5—C3—C4	123.1 (5)	C8—C9—C4	123.2 (5)
O5—C3—C2	120.6 (7)	C11—C10—C15	118.1 (6)
C4—C3—C2	116.3 (6)	C11—C10—C1	121.3 (6)
C9—C4—C3	120.2 (5)	C15—C10—C1	120.6 (7)
C9—C4—C5	116.4 (6)	C10—C11—C12	121.5 (7)
C3—C4—C5	123.4 (5)	C11—C12—C13	119.4 (8)
O6—C5—C6	120.0 (5)	C14—C13—O2	125.2 (6)
O6—C5—C4	117.6 (7)	C14—C13—C12	120.6 (6)
C6—C5—C4	122.4 (5)	O2—C13—C12	114.2 (7)

Table 3. Dihedral angles (°) between rings *A* and *C*, and rings *B* and *C*, and the shift (*S*, Å) of the center of ring *B* from the plane of ring *C* for flavone molecules

Compound	<i>A</i> [∧] <i>C</i>	<i>B</i> [∧] <i>C</i>	<i>S</i>	References
Flavocommelin octaacetate	1.6 (2)	6.2 (3)	0.25 (2)	This work
6-Hydroxyflavone	2.3 (2)	9.8 (2)	0.01 (2)	Seetharaman & Rajan (1992)
Artemetin	2.0 (3)	1.2 (3)	0.03 (2)	Estrada, Conde, Ma'rquez & Jimenez-Garay (1987)
4'-Methoxyflavone	1.1 (1)	2.2 (1)	0.03 (1)	Wallet, Gaydou, Tinant, Declercq & Baldy (1991)
4'-Fluorobenzofl[avone]	2.0 (1)	2.2 (1)	0.05 (1)	Neuman <i>et al.</i> (1989)
Calycopterin	3.1 (5)	18.6 (6)	0.06 (1)	Vijayalakshmi, Rajan, Srinivasan & Ramachandran Nair (1986)
Gardenin A	1.1 (4)	24.8 (4)	0.06 (1)	Vijayalakshmi, Rajan & Srinivasan (1987)
4'-Methoxybenzofl[avone]	2.6 (1)	2.5 (1)	0.13 (1)	Neuman <i>et al.</i> (1989)
6,2',3',4'-Tetramethoxyflavone	1.8 (1)	45.0 (1)	0.13 (1)	Wallet <i>et al.</i> (1990)
Prudomestin	1.8 (2)	3.8 (2)	0.14 (1)	Parmar, Vardhan, Sharma, Alcock & Errington (1992)
5-Hydroxybenzofl[avone]	0.3 (1)	9.4 (1)	0.15 (1)	Neuman <i>et al.</i> (1989)
Flavone hymenoxin	4.4 (4)	4.4 (1)	0.17 (1)	Watson, Kashyap, Gao & Mabry (1991)
3',4'-Dimethoxyflavone	1.5 (1)	6.2 (1)	0.18 (1)	Wallet, Gaydou, Tinant, Declercq & Baldy (1991)
2',7'-Dimethoxyflavone	2.5 (1)	24.3 (1)	0.26 (1)	Wallet, Gaydou, Feneau-Dupont, Tinant, Declercq & Baldy (1991)
Aciculatin (molecule <i>A</i>)	1.2 (3)	13.8 (4)	0.09 (3)	Krause & Eggleston (1991)
(molecule <i>B</i>)	3.3 (3)	17.8 (3)	0.09 (2)	
6-(4- <i>n</i> -Propoxybenzoyloxy)-flavone (molecule <i>A</i>)	1.3 (1)	9.8 (1)	0.17 (1)	Kawai, Yoshimura, Shimaoka, Nakamura & Yano (1991)
(molecule <i>B</i>)	2.2 (1)	5.3 (1)	0.15 (1)	
(molecule <i>C</i>)	0.5 (1)	14.6 (1)	0.08 (1)	

Determination of lattice parameters and preliminary X-ray intensity measurement were carried out on an automated AFC-5 four-circle diffractometer with graphite-monochromated Mo *K*α radiation. The X-ray diffraction data were measured using a Weissenberg camera for macromolecular crystallography (Sakabe, 1991) with imaging plates at BL-6A₂, Photon Factory, KEK. A camera of radius 143.0 mm was used with an imaging plate of 200 × 400 mm. The observable 2θ range was from -70 to 90° in the radial direction and ±35° in the axial direction of the cassette. The needle axis (*c*) was the rotation axis. Polychromatic synchrotron radiation was monochromated by an Si(111) single monochromator. Reflections with $\sin\theta/\lambda < 0.668 \text{ \AA}^{-1}$ were processed, scaled and then merged. The overall merging $R(F^2)$ factor was 0.075. The strong low-order reflections were overloaded during read-out of imaging plates because of the dynamic range of the scanner system (BA100, Fuji Photo Film Co. Ltd) and 209 reflections were replaced with those measured with Mo *K*α radiation after scaling. The agreement factor on *F* between the synchrotron and Mo *K*α data [$|F_o| > 20\sigma(|F_o|)$] was 0.015 for 152 independent reflections. The absolute structure was assigned based on the absolute configuration of D-(+)-glucose. Calculations were carried out using *CRYSTAN-GM* software (MAC Science, 1992) on a SUN SPARC2 workstation at Keio university.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71626 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1047]

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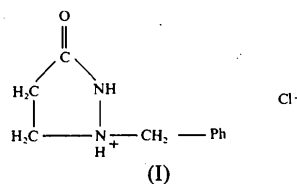
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of the cation has an approximate half-chair conformation. Atom N(1) is *sp*³ hybridized while atom N(2) is *sp*² hybridized. The C(3)—N(2) bond distance of 1.373 (4) Å is a partial double bond. Both H atoms connected to N atoms are involved in hydrogen bonding of the N—H...Cl type.

Comment

γ-Aminobutyrate (GABA) is known to be a depressant neurotransmitter. Therefore, an increase in the GABA content of the brain might be correlated with anticonvulsant activity. Since 3-pyrazolidones were reported to be a potent inhibitor of GABA-transaminase (White *et al.*, 1982), these kinds of compounds have been expected to be effective in elevating GABA levels in the brain and correspondingly to have anticonvulsant activity. Pharmacological tests have proved that expectation (Ling, Li, Liu & Pei, 1986; Du, Ling, Liu, Ku & Liu, 1989; Lei, Luan, Ling, Li & Pei, 1990; Lei, Zhang, Ling & Ku, 1990). The X-ray analysis of the title compound was undertaken as part of a search for common conformational features of 3-pyrazolidones, which may help in understanding the mechanism of action of such compounds at the molecular level, as well as providing a reliable molecular model for 3D-QSAR comparative molecular-field analysis.

According to the results of structural analysis, the crystal structure of the title compound (I) consists of cations of protonated 1-benzyl-3-pyrazolidone and chloride anions. This indicates that the lone pair of electrons on atom N(1) is clearly protophilic. Fig. 1 provides a view of the structural features of the cation.



The conformation of the five-membered ring is approximately a half-chair; atoms N(1) and C(5) are displaced on opposite sides of the plane through atoms N(2), C(3), C(4) and O (planar within 0.006 Å) with displacements of 0.264 and 0.220 Å, respectively. Examination of the intramolecular bond angles associated with atoms N(1) and N(2) suggests that N(1) is *sp*³ hybridized, displaying bond angles N(2)—N(1)—C(5) 103.2 (2), N(2)—N(1)—C(6) 111.4 (2), C(5)—N(1)—C(6) 116.0 (2) and N(2)—N(1)—H(N1) 106 (2)°, while N(2) is approximately *sp*² hybridized. The sum of the bond angles about atom N(2) is 351.0°. The C(3)—N(2) bond distance

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1-Benzyl-3-pyrazolidone Hydrochloride

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Abstract

The crystal of the title compound, C₁₀H₁₃N₂O⁺.Cl⁻, consists of 1-benzyl-3-oxo-1*H*⁺-pyrazolidinium cations and chloride anions. The five-membered ring