

Note

Synthesis and Crystal Structure of a Novel Supramolecular Compound $[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}$

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A hydrolyte of magnesium 7-methoxy-4'-hydroxyisoflavone-3'-sulfonate ($[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}$) was synthesized and its crystal structure was determined by X-ray diffraction analyses. The crystal belongs to triclinic crystal system, space group *P*-1 with cell constants $a = 0.7359$ (1) nm, $b = 0.9935$ (1) nm, $c = 1.6335$ (2) nm, $\alpha = 91.16$ (1)°, $\beta = 92.07$ (1)°, $\gamma = 106.53$ (1)°, $V = 1.1436$ (2) nm³ and $Z = 1$. The results show that the title compound consists of $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$, $\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3^-$ and H_2O . Mg(II) is located at the symmetry center of the title compound. $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$, $\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3^-$ and H_2O form fourteen kinds of hydrogen bonds. The distance of 0.351 nm between parallel isoflavone rings shows a π - π stacking interaction. The hydrogen bonds and π - π stacking interaction lead to supramolecular formation with three-dimensional network structure. The title compound was also characterized by IR and ¹H NMR spectra.

Keywords daidzein, isoflavone, hydrolyte of magnesium 7-methoxy-4'-hydroxyisoflavone-3'-sulfonate, crystal structure, supramolecular, hydrogen bonds

Introduction

Molecular polymer with one dimensional or multidimensional structure assembling through hydrogen bonds is an important research content in the supramolecular chemistry and crystal engineering.^{1,2} With the development of new type functional materials such as molecular magnetic, selected catalysis, reversible catalysis, reversible host-guest molecular (ion) exchange etc.,³ the molecular design and synthesis have already attracted considerable attention in supramolecular system. The supramolecular complexes and organic compounds containing hydrogen bond have also been extensively studied.^{4,6}

Daidzein (4', 7-dihydroxy-isoflavone) is one of effects principal of soy isoflavone. It has been pharmacologically shown with the effects of antidysrhythmic,⁷ antioxidant,^{8,9} getting rid of hyperkinesias,¹⁰ inhibiting cancer cells growth,¹¹⁻¹³ accelerating the formation of bone cells¹⁴ and

playing a role of female hormone.¹⁵ Because the solubility of daidzein is poor, its biological utilization rate is lower and the dose of daidzein is more.¹⁶ We thus require a route to synthesize a water soluble derivative of daidzein in order to study its possible biological effects. In this paper, the synthesis and crystal structure of a novel hydrolyte of magnesium 7-methoxy-4'-hydroxyisoflavone-3'-sulfonate ($[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}$) was reported. The crystal structure shows that $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$, $\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3^-$ and H_2O form fourteen kinds of hydrogen bonds. The distance of 0.351 nm between parallel isoflavone rings shows a π - π stacking interaction. The hydrogen bonds and π - π stacking interaction lead to supramolecular formation with three-dimensional network structure. The preparation of the title compound can be expressed as Scheme 1.

Experimental

Synthesis of the title compound

Chemicals were of analytical reagent grade and were used directly without further purification. The infrared spectra were recorded as KBr pellets on a Nicolet 170SX FT-IR spectrometer. The ¹H NMR spectra were recorded on a Bruker AM-400 spectrometer with TMS as internal reference and $\text{DMSO}-d_6$ as solvent. C and H contents were analyzed using a PE-2400 elemental analytic instrument.

7-Methoxy-4'-hydroxyisoflavone was prepared with daidzein according to the reported method.¹⁴ 7-Methoxy-4'-hydroxyisoflavone (6.5 g) was slowly added to 98% sulfuric acid (52 mL) with stirring. The mixture was heated at 60 °C for half an hour and cooled at room temperature. After being cooled, the above reaction mixture was added to an aqueous solution of saturated sodium chloride (350 mL) and colorless of precipitation began to appear. After 4 h, the precipitate was filtered and washed with saturated sodium chloride solu-

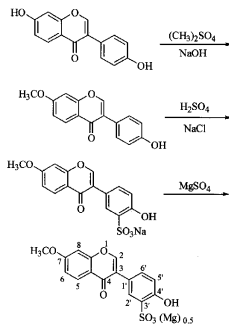
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tion until the pH of filtrate was 6–7. The precipitate was dissolved in water (100 mL), and was mixed with 10% $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ solution (40 mL). The crystals of the title compound were obtained after 24 h and recrystallized in water to give product in good yield (79%). Colorless plate single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of its water solution. M. p. 295.4 °C (decompose). Anal. calcd for $\text{C}_{32}\text{H}_{34}\text{MgO}_{10}\text{S}_2$: C 38.13, H 5.36; found C 38.05, H 5.33. IR spectra shows that the bonds are as follows; 3405 (br s), 2984 (s), 2899 (s), 1632 (s), 1561 (m), 1504 (m), 1443 (m), 1273 (m), 1207 (br s), 1169 (m) cm^{-1} . The strongest peaks at 1632 cm^{-1} and 1207 cm^{-1} belong to the $-\text{C}=\text{O}^{20}$ and $-\text{SO}_3^{21}$ vibration of the group in the isoflavone skeleton, respectively. NMR spectra are as follows: ^1H NMR (DMSO- d_6 , 400 MHz) δ : 8.42 (s, 1H, H-C₂), 8.04 (d, $J=9.2$ Hz, 1H, H-C₇), 7.09 (dd, $J=9.2, 2.4$ Hz, 1H, H-C₆), 7.19 (d, $J=2.4$ Hz, 1H, H-C₈), 3.91 (s, 3H, H₃CO), 7.69 (d, $J=2.0$ Hz, 1H, H-C_{2'}), 7.41 (dd, $J=8.4, 2.0$ Hz, 1H, H-C_{6'}), 6.84 (d, $J=8.4$ Hz, 1H, H-C_{7'}), 10.63 (s, 1H, HO-C_{4'}).

Scheme 1



X-Ray crystal structure determination

The crystal used for X-ray determination was obtained as described in preparation section. The sample selected for investigation has dimensions of 0.44 mm \times 0.30 mm \times 0.24 mm. The data were collected with graphite monochromated Mo K α radiation ($\lambda = 0.071073$ nm) using a siemens P4 four-circle diffractometer. A total of 5443 reflections were collected to give 4038 independent reflections ($R_{\text{int}} = 0.0327$). The structure was solved using direct meth-

ods with SHELXTL program and refined by full-matrix least-squares techniques. The non-hydrogen atoms were assigned anisotropic displacement parameters in the refinement. The hydrogen atoms were treated using a riding model. The structure was then refined on F^2 using SHELXTL-97. The final R value (on F) was 0.0621. The crystal and refinement data are listed in Table 1. The fractional non-hydrogen atomic coordinates and equivalent isotropic displacement parameters are shown in Table 2. Selected bond lengths and angles are given in Table 3.

Table 1 Crystal data and details of the structure determination for $[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}$

Empirical formula	$\text{C}_{32}\text{H}_{34}\text{MgO}_{10}\text{S}_2$
Formula weight	1007.18
Temperature	295(2) K
Crystal system	Triclinic
Space group	$P-1$
Unit cell dimensions	$a = 0.7359(1)$ nm, $a = 91.16(1)^\circ$ $b = 0.9935(1)$ nm, $\beta = 92.07(1)^\circ$ $c = 1.6335(2)$ nm, $\gamma = 106.53(1)^\circ$
Volume, Z	1.1436(2) nm 3 , 1
Density (calculated)	1.462 g/cm 3
Absorption coefficient	0.228 nm $^{-1}$
$F(000)$	530
Crystal size	0.44 mm \times 0.30 mm \times 0.24 mm
θ Range for data collection	2.14 to 25.00 $^\circ$
Limiting indices	$0 \leq h \leq 8$, $-11 \leq k \leq 11$, $-19 \leq l \leq 19$
Reflections collected	5443
Independent reflections	4038 [$R_{\text{int}} = 0.0327$]
Max. and min. transmission	0.9828 and 0.9271
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4038/20/337
Goodness-of-fit on F^2	0.994
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0621$, $\omega R_2 = 0.1741$
R indices (all data)	$R_1 = 0.0932$, $\omega R_2 = 0.1908$
Extinction coefficient	0.003(3)
Largest diff. peak and hole	1229 and -527 e $^-$ /nm 3

Results and discussion

The molecular structure and packing diagram of the title compound are shown in Fig. 1 and Fig. 2, respectively. The title compound consists of a complex cation $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$, a sulfonate of isoflavone anion $\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3^-$ and ten lattice water molecules. Mg^{2+} cation is located at the symmetry center of $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$ and coordinated by six water molecules. $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$, of which the average $\text{Mg}-\text{O}$ bond length is 0.204 nm, is a slightly distorted octahedral complex cation. In the anion, the geometry of isoflavone skeleton is similar to that of its analogues such as dalspinin,¹⁸ as well as most of the bonds and bond angles. The atoms of ring A ($\text{C}_{10}-\text{C}_{15}$) and ring C (C_7-C_{11}) of

isoflavone are nearly in a plane, the dihedral angle between ring A and ring C systems is 3.4° . To avoid steric conflicts, ring B (C_1-C_6) and ring C two rigid ring systems are rotated by 61.5° with respect to each other.

Table 2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{nm}^2 \times 10$)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}^a
Mg	10000	5000	0	40(1)
S	6225(1)	6279(1)	2018(1)	42(1)
O(1)	3114(4)	7581(3)	2124(2)	50(1)
O(2)	2662(4)	2500(3)	5724(2)	52(1)
O(3)	2214(4)	1479(3)	3280(2)	52(1)
O(4)	2824(5)	-2096(3)	6405(2)	63(1)
O(5)	5416(4)	6027(3)	1187(2)	57(1)
O(6)	7416(4)	5391(4)	2222(2)	63(1)
O(7)	7137(4)	7760(3)	2172(2)	61(1)
O(8)	7495(5)	5487(6)	-76(2)	91(1)
O(9)	11286(8)	6989(4)	437(3)	106(2)
O(10)	10349(5)	5622(4)	-1195(2)	64(1)
O(11)	8276(5)	7422(4)	-1694(2)	70(1)
O(12)	10769(7)	9143(5)	-472(3)	99(1)
O(13)	5186(7)	7879(6)	-799(3)	117(2)
O(14)	5690(9)	9385(5)	865(3)	122(2)
O(15)	904(4)	9150(3)	2227(2)	66(1)
C(1)	2935(5)	6551(4)	2269(2)	38(1)
C(2)	1462(5)	6160(4)	3190(2)	42(1)
C(3)	1345(5)	5077(4)	3726(2)	42(1)
C(4)	2720(5)	4363(4)	3754(2)	39(1)
C(5)	4186(5)	4739(4)	3214(2)	38(1)
C(6)	4316(5)	5821(4)	2685(2)	35(1)
C(7)	2712(6)	3457(4)	5145(2)	47(1)
C(8)	2624(5)	3214(4)	4334(2)	41(1)
C(9)	2417(5)	1783(4)	4023(2)	39(1)
C(10)	2457(5)	773(4)	4646(2)	39(1)
C(11)	2597(5)	1161(4)	5467(2)	40(1)
C(12)	2714(6)	269(4)	6092(2)	46(1)
C(13)	2672(6)	-1087(4)	5870(2)	48(1)
C(14)	2514(6)	-1528(4)	5044(3)	51(1)
C(15)	2415(6)	-615(4)	4449(2)	46(1)
C(16)	3064(9)	-1706(6)	7261(3)	81(2)

^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

In the crystal structure, the sulfo-group ($-SO_3$), carbonyl ($-C=O$), hydroxyl ($-OH$) of the isoflavone skeleton, the ten lattice water molecules and the six coordinated water molecules are linked by fourteen kinds of hydrogen bond. The typical hydrogen bond lengths and angles are given in Table 4. The hydrogen bonds can be classed in four types.

The first type is the hydrogen bonds between $[Mg(H_2O)_6]^{2+}$ and $C_{16}H_{11}O_4SO_3^-$, including 4 kinds of hydrogen bonds. $O(8)-H(8A)\cdots O(5)$, $O(10)-H(10A)\cdots O(6)$ and $O(8)-H(8B)\cdots O(5)$ hydrogen bonds exist between coordinated water molecules and sulfo-group, $O(9)-$

$H(9B)\cdots O(1)$ hydrogen bonds exist between coordinated water molecule and 4'-hydroxyl. The second type hydrogen bonds consists of five kinds of hydrogen bonds between $C_{16}H_{11}O_4SO_3^-$ and lattice water molecules. $O(1)-H(10)\cdots O(15)$, $O(14)-H(14A)\cdots O(1)$ hydrogen bonds exist between 4'-hydroxyl and lattice water molecules. $O(11)-H(11B)\cdots O(3)$, $(15)-H(15A)\cdots O(3)$ hydrogen bonds exist between carbonyl and lattice water molecules. $O(15)-H(15B)\cdots O(7)$ is the hydrogen bonds between the oxygen atom of sulfo-group and lattice water molecules. $O(10)-H(10B)\cdots O(11)$, $O(9)-H(9A)\cdots O(12)$ hydrogen bonds are the third type hydrogen bonds, they exist between coordinated water molecules and lattice water molecules. The hydrogen bonds between lattice water molecules are the fourth type hydrogen bonds, including $O(12)-H(12A)\cdots O(11)$, $O(11)-H(11A)\cdots O(13)$ and $O(14)-H\cdots O(13)$ hydrogen bonds. In the above hydrogen bonds, the strongest one exists between the H atom of 4'-hydroxyl and the O(15) atom of lattice water molecule, and its bond length is 0.178 nm. It should also be pointed out that these hydrogen bonds (and/or, interaction) not only connect the cations with anions together to form three-dimensional network structure, but also play very important roles in the formation, stability and crystallization of the title compound.

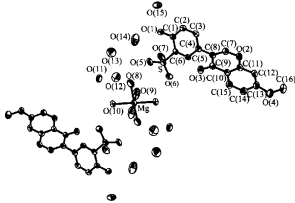


Fig. 1 Molecular structure of the title compound.

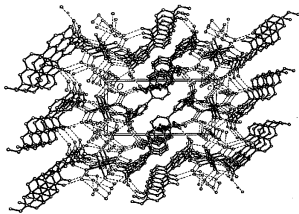


Fig. 2 Unit cell packing diagram of the title compound.

Table 3 Selected bond lengths (nm) and angles ($^{\circ}$) for $[\text{Mg}(\text{H}_2\text{O})_6]_2(\text{C}_{16}\text{H}_{11}\text{O}_4\text{S}_3)_2 \cdot 10\text{H}_2\text{O}$

Bond distances			
Mg—O(8)	0.2035(3)	Mg—O(9)	0.2035(4)
Mg—O(10)	0.2063(3)	S—O(5)	0.1451(3)
S—O(6)	0.1445(3)	S—O(7)	0.1446(3)
S—C(6)	0.1770(4)	O(1)—C(1)	0.1352(4)
O(2)—C(7)	0.1348(5)	O(2)—C(11)	0.1373(5)
O(3)—C(9)	0.1237(4)	O(4)—C(13)	0.1368(5)
O(4)—C(2)	0.1434(6)	C(1)—C(2)	0.1375(5)
C(1)—C(6)	0.1406(5)	C(2)—C(3)	0.1387(5)
C(3)—C(4)	0.1391(5)	C(4)—C(5)	0.1391(5)
C(4)—C(8)	0.1486(5)	C(5)—C(6)	0.1377(5)
C(7)—C(8)	0.1337(5)	C(8)—C(9)	0.1465(5)
C(9)—C(1)	0.1449(5)	C(10)—C(1)	0.1381(5)
C(10)—C(2)	0.1402(5)	C(11)—C(1)	0.1381(5)
C(12)—C(1)	0.1380(6)	C(13)—C(1)	0.1400(6)
C(14)—C(2)	0.1357(6)		
Bond angles			
O(8)—Mg—O(8) # 1	180.0(3)	O(8)—Mg—O(9)	88.9(2)
O(8) # 1—Mg—O(9)	91.1(2)	O(8)—Mg—O(9) # 1	91.1(2)
O(8) # 1—Mg—O(9) # 1	88.9(2)	O(9)—Mg—O(9) # 1	180.0(2)
O(8)—Mg—O(10) # 1	93.4(1)	O(8) # 1—Mg—O(1) # 1	86.62(1)
O(9)—Mg—O(10) # 1	88.5(2)	O(9) # 1—Mg—O(10) # 1	91.5(2)
O(8)—Mg—O(10)	86.6(1)	O(8) # 1—Mg—O(10)	93.4(1)
O(9)—Mg—O(10)	91.54(2)	O(9) # 1—Mg—O(10)	88.5(2)
O(10) # 1—Mg—O(10)	180.0(2)	O(6)—S—O(7)	113.9(2)
O(6)—S—O(5)	112.8(2)	O(7)—S—O(5)	110.4(2)
O(6)—S—C(6)	105.9(2)	O(7)—S—C(6)	106.1(2)
O(5)—S—C(6)	107.2(2)	C(7)—O(2)—C(11)	117.8(3)
C(13)—O(4)—C(16)	117.3(4)	O(1)—C(1)—C(2)	123.7(3)
O(1)—C(1)—C(6)	117.7(3)	C(1)—C(2)—C(3)	120.8(3)
C(2)—C(3)—C(4)	120.9(3)	C(5)—C(4)—C(8)	120.5(3)
C(3)—C(4)—C(8)	121.4(3)	C(6)—C(5)—C(4)	121.1(3)
C(5)—C(6)—S	119.5(3)	C(1)—C(6)—S	120.1(3)
C(8)—C(7)—O(2)	126.0(4)	C(7)—C(8)—C(9)	118.7(4)
C(7)—C(8)—C(4)	121.1(3)	O(9)—C(8)—C(4)	120.1(3)
O(3)—C(9)—C(10)	123.4(3)	O(3)—C(9)—C(8)	121.6(3)
C(11)—C(10)—C(15)	117.0(4)	C(11)—C(10)—C(9)	120.7(3)
C(15)—C(10)—C(9)	122.2(3)	O(2)—C(11)—C(10)	121.5(3)
O(2)—C(11)—C(12)	114.6(3)	C(10)—C(11)—C(12)	123.8(4)
C(13)—C(12)—C(11)	117.2(4)	O(4)—C(13)—C(12)	125.1(4)
C(12)—C(13)—C(14)	120.8(4)	C(15)—C(14)—C(13)	120.1(4)
C(14)—C(15)—C(10)	121.1(4)		

Symmetry code " # 1": $-x+2, -y+1, -z$

In the title compound, the isoflavone skeleton of anions are linked layer by layer, the neighboring layers are connected through the hydrogen bonds of $\text{O}(1)\cdots\text{H}(10)\cdots\text{O}(15)$

and $\text{O}(15)\cdots\text{H}(15\text{B})\cdots\text{O}(7)$. Furthermore, the rings of two isoflavone structures are stacking, their arrangement is as follows:

Table 4 Typical hydrogen bond lengths (nm $\times 10^{-1}$) and bond angles ($^{\circ}$) for $[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}^a$

Bond	O—H	H...O	Distance	Angle
O(1)—H(10)···O(15)	0.820	1.780	2.560(4)	158.0
O(8)—H(8A)···O(5)	0.820(1)	1.938(9)	2.744(4)	168(4)
O(11)—H(11A)···O(13)	0.820(1)	2.082(1)	2.883(6)	165(4)
O(10)—H(10B)···O(11)	0.820(1)	1.985(2)	2.777(5)	162(5)
O(9)—H(9A)···O(12)	0.820(1)	1.956(2)	2.735(6)	158(4)
O(12)—H(12A)···O(11)	0.820(1)	2.050(2)	2.844(6)	163(2)
O(14)—H(14A)···O(1)	0.820(1)	2.380(3)	3.087(5)	144(5)
O(15)—H(15A)···O(3)	0.820(1)	1.961(7)	2.773(4)	171(4)
O(15)—H(15B)···O(7)	0.820(1)	1.914(2)	2.720(4)	167(8)
O(9)—H(9B)···O(1)	0.820(1)	2.193(2)	2.993(5)	165(5)
O(8)—H(8B)···O(5)	0.820(1)	2.140(3)	2.814(5)	139(5)
O(11)—H(11B)···O(3)	0.820(1)	2.150(3)	2.882(4)	149(6)
O(10)—H(10A)···O(6)	0.820(1)	2.000(3)	2.757(4)	153(5)
O(14)—H(14B)···O(13)	0.820(1)	2.300(3)	3.036(7)	150(6)

^a The A and B are two hydrogen atoms from the same water molecule.



Where, A, C or C, A in a line expresses ring A (C_{10} — C_{15}) and ring C (C_7 — C_{11}) of a same isoflavone skeleton. In the crystal structure, a stacking interaction exists between ring A, ring C of an isoflavone skeleton and ring C, ring A of another isoflavone skeleton, respectively, their distance is 0.356 nm. Another stacking interaction exists between ring A of an isoflavone skeleton and ring A of another isoflavone skeleton, their distance is 0.351 nm. Obviously, both of the distances are shorter than that of π ··· π stacking interactions (0.366—0.380 nm) which was reported by Zheng *et al.*,¹⁹ this fact indicates that a stronger π ··· π stacking interaction exists between the rings of isoflavone skeletons in the crystal of $[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}$.

In the crystal of the title compound, fourteen kinds of hydrogen bonds between sulfo-group ($-\text{SO}_3^-$), carbonyl ($-\text{C}=\text{O}$), hydroxyl ($-\text{OH}$) of the isoflavone skeleton, lattice water molecules, coordinated water molecules and the π ··· π stacking interactions of isoflavone skeletons and the electrostatic interaction between the cation $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$ and the anion sulfonate $\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3^-$ lead to the moieties into a supramolecule of three-dimensional structure. It is interesting that the novel supramolecular compound has a special packing manner. In Fig. 2, coordinated water molecules, sulfo-group, carbonyl and phenol hydroxyl, they are hydrophilic. The distance between them is small. The areas which are surrounded by the hydrophilic group are filled with the lattice water molecules, therefore, there are hydrogen

bonds network in the areas. On the contrary, there is not any hydrophilic group and hydrogen bond in the areas which are surrounded by two isoflavone structures. This area is like a cave in the crystal of $[\text{Mg}(\text{H}_2\text{O})_6](\text{C}_{16}\text{H}_{11}\text{O}_4\text{SO}_3)_2 \cdot 10\text{H}_2\text{O}$, the reason can be explained as the absence of hydrophilic groups.

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