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Pyridinium 4-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]-benzenesulfonate

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.130
Data-to-parameter ratio = 11.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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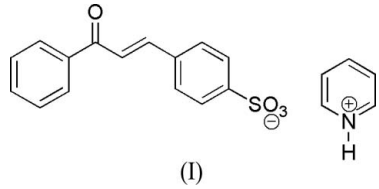
In the title compound, $C_5H_6N^+\cdot C_{15}H_{11}O_4S^-$, the C—C—C—C torsion angle of −166.9 (2)° between the 5-vinylbenzenesulfonate group and the phenyl ring indicates the nonplanarity of the system. The NH group of the pyridinium ring has an intermolecular contact with a sulfonyl O atom. Six intermolecular C—H···O hydrogen bonds are also observed in the crystal structure.

Comment

Chalcones are natural compounds of the flavonoid family. Chemically, they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β-unsaturated carbonyl system. They exhibit biological activities, the most important being oestrogenic, antifungal, antinociceptive, antibacterial, antiviral and antiflammatory (Dimmock *et al.*, 1999). Their antifungal and antileishmanial activities suggest that the mode of action of some chalones is by inhibiting the activity of an enzyme that participates in the biosynthesis of ergosterol (Chan-Bacab & Pena-Rodriguez, 2001). We have investigated a series of novel synthetic chalcone derivatives for their trypanocidal and leishmanicidal properties (Lunardi *et al.*, 2003; Andrighetti-Fröhner *et al.*, 2003). In the light of this interest, we report here the crystal structure of the title compound, (I).



(I)

In (I), the 5-vinylbenzenesulfonate group is nearly planar, with a deviation from the mean plane of 0.112 (2) Å for C7 and −0.096 (2) Å for C8. The C7—C8—C9—C10 torsion angle of −166.9 (2)° between this group and the phenyl ring indicates the nonplanarity of the system. The C6—H6···O1^{v}═S1^{v} and C3—H3···O4^{vi}═C9^{vi} hydrogen bonds build bilayers of 4-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]benzenesulfonate anions perpendicular to the *a* axis and connected by a layer of pyridinium cations by the hydrogen bonds N1—H1*N*···O3^{i}═S1^{i}, C16—H16···O1^{ii}═S1^{ii}, C20—H20···O1^{i}═S1^{i}, C17—H17···O2^{iv}═S1^{iv} and C19—H19···O2^{iii}═S1^{iii}. Details of the hydrogen bonding, including symmetry codes, are given in Table 1.

Experimental

The title compound (I) was prepared according to the literature procedure (da Silva *et al.*, 2006). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from a methanol–dichloromethane solution (1:1).

Crystal data

$C_5H_6N^+\cdot C_{15}H_{11}O_4S^-$
M_r = 367.41
Monoclinic, $P2_1/c$
a = 17.034 (2) Å
b = 9.0682 (9) Å
c = 11.832 (2) Å
β = 96.61 (2)°
V = 1815.5 (4) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.80 mm^{-1}
T = 299 (2) K
0.50 × 0.40 × 0.35 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3698 measured reflections
3222 independent reflections
2812 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.09
3222 reflections
287 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O3^{i}	0.97 (3)	1.86 (3)	2.790 (2)	159 (3)
C16—H16···O1^{ii}	0.88 (3)	2.44 (3)	3.260 (3)	156 (2)
C19—H19···O1^{iii}	0.95 (3)	2.42 (3)	3.324 (3)	161 (2)
C17—H17···O2^{iv}	1.00 (3)	2.48 (3)	3.224 (3)	132 (2)
C20—H20···O2^{i}	0.92 (3)	2.52 (3)	3.251 (3)	136 (2)
C6—H6···O1^{v}	0.93 (3)	2.40 (3)	3.303 (3)	164 (2)
C3—H3···O4^{vi}	0.93 (3)	2.42 (3)	3.275 (3)	152 (2)

Symmetry codes: (i) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y, -z+1$; (v) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (vi) $-x+1, -y+1, -z+1$.

H atoms were located in difference maps and their positions refined [C—H = 0.87 (3)–1.01 (4) Å, N—H = 0.97 (3) Å), with U_{iso}(H) = 1.2U_{eq}(parent atom)].

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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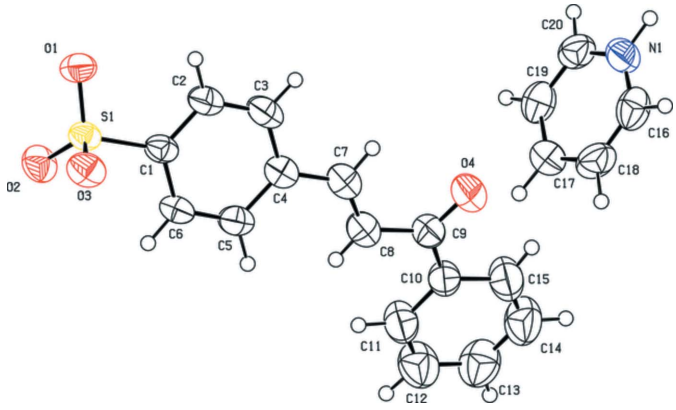

Figure 1
The molecular structure of (I), with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

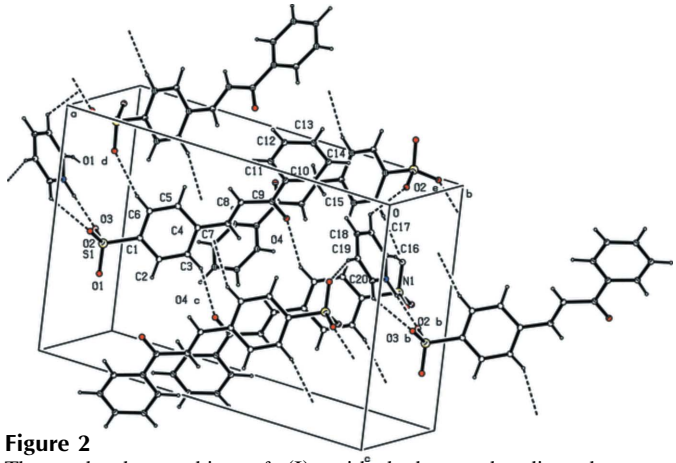

Figure 2
The molecular packing of (I), with hydrogen bonding shown as dashed lines. [Symmetry codes: (*b*) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (*c*) $-x+1, -y+1, -z+1$; (*d*) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (*e*) $-x+1, -y, -z+1$.]

References

Andrighetti-Fröhner, C. R., Antonio, R. V., Creczynski-Pasa, T. B., Barardi, C. R. & Simões, C. M. O. (2003). *Mem. Inst. Oswaldo Cruz*, **98**, 843–848.
Chan-Bacab, M. J. & Pena-Rodriguez, L. M. (2001). *Nat. Prod. Rep.* **18**, 674–688.
Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. M. (1999). *Curr. Med. Chem.* **6**, 1125–1149.
Enraf–Nonius (1996). *CAD-4-PC*. Version 1.2. Enraf–Nonius, Delft, The Netherlands.
Lunardi, F., Guzela, M., Rodriguez, A. T., Corrêa, R., Eger-Mangrich, I., Steindel, M., Grisard, E. C., Assreuy, J., Calixto, J. B. & Santos, A. (2003). *Antimicrob. Agents Chemother.* **47**, 1449–1451.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Silva, L. E. da, Andrighetti-Fröhner, C. R., Nunes, R. J., Simões, C. M. O. & Foro, S. (2006). *Acta Cryst.* E**62**, o2104–o2105.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.