Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Kumar, S., Wilson, S. R. & Leonard, N. J. (1988). *Acta Cryst.* C**44**, 508–510.
Munns, A. R. I. & Tollin, P. (1970). *Acta Cryst.* B**26**, 1101–1113.
Schmalle, H. W., Hänggi, G. & Dubler, E. (1988). *Acta Cryst.* C**44**, 732–736.
Shefter, E. & Trueblood, K. N. (1965). *Acta Cryst.* **18**, 1067–1077.
Sheldrick, G. M. (1976). *SHELX76*. A program for crystal structure determination. Univ. of Cambridge, England.
Sheldrick, G. M. (1985). *SHELX86*. In *Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 175–189. Oxford Univ. Press.
Thewalt, U., Bugg, C. E. & Marsh, R. E. (1970). *Acta Cryst.* B**26**, 1089–1101.
Tindall, C. G. Jr, Robins, R. K., Tolman, R. L. & Hutzenlaub, W. (1972). *J. Org. Chem.* **37**, 3985–3989.
Woese, C. R. (1967). In *The Genetic Code*. New York: Harper & Row.
Wolfenden, R., Sharpless, T. K., Ragade, I. S. & Leonard, N. J. (1966). *J. Am. Chem. Soc.* **88**, 185–186.

Acta Cryst. (1989). C**45**, 1397–1400

Structures of Two Dimers Obtained by Hydrogenation of the Methyl and Trimethyl Derivatives of Hydroxyflavylium Chloride

By Lahcène Ouahab,* Abdelhamid Mousser, Ali Boultif and Daniel Grandjean

Laboratoire de Chimie du Solide et Inorganique Moléculaire, UA CNRS 254, *Université de Rennes* I,
35042 *Rennes CEDEX, France*

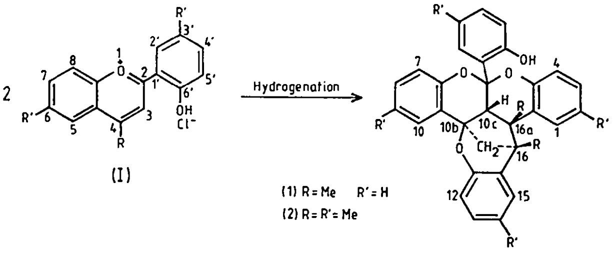
and Henri Jolibois

Département de Chimie, Faculté des Sciences, Route de Gray, 25030 *Besancon CEDEX, France*

(*Received* 20 *September* 1988; *accepted* 31 *January* 1989)

Abstract. (1) 2-[4b,5,10a,15b-Tetrahydro-5,10a-methano-4b,5-dimethyl-5a*H*-di[1](benzopyrano)-[4,3-*b*:3′,4′-*c*;2,3:2′,3′][1]benzoxepin-15a-yl]phenol acetone solvate, $C_{32}H_{26}O_4.C_3H_6O$, M_r = 532·64, triclinic, $P\bar{1}$, a = 10·104 (8), b = 10·981 (7), c = 14·437 (7) Å, α = 91·76 (4), β = 106·21 (3), γ = 110·62 (4)°, V = 1424·7 Å^3, Z = 2, D_x = 1·24 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 0·77 cm^{-1}, $F(000)$ = 564, T = 293 K, R = 0·054 based on 2828 observed reflections with $I \geq 3\sigma(I)$. (2) 4-Methyl-[4b,5,10a,15b-tetrahydro-5,-10a-methano-3,4b,5,7,12-pentamethyl-5a*H*-di[1]-(benzopyrano)[4,3-*b*:3′,4′-*c*,-2,3:2′,3′][1]benzoxepin-5a-yl]phenol ethyl acetate solvate, $C_{36}H_{34}O_4.C_4H_8O_2$, M_r = 618·78, monoclinic, $P2_1/c$, a = 10·10·551 (6), b = 19·881 (4), c = 16·446 (8) Å, β = 104·49 (5)°, V = 3339·9 Å^3, Z = 4, D_x = 1·23 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 0·76 cm^{-1}, $F(000)$ = 1320, T = 293 K, R = 0·050 based on 2994 observed reflections with $I \geq 3\sigma(I)$. The compounds are formed by the association of two flavane skeletons. This association is established at three points (C7⋯C18, O3⋯C16 and C9⋯C17) and results in the formation of a five-membered ring and a heterocycle. All the junction C atoms are sp^3 hybridized and the molecules are not planar.

Introduction. Few examples of the reduction of flavylium salts have appeared in the literature (Reynolds, Van Allan & Regan, 1967; Reynolds & Van Allan, 1967; Jurd & Roitman, 1978). These structures are assigned on the basis of the NMR, IR and mass spectra. We have reported recently a procedure used for the reduction of 2′-hydroxy-4′-methylflavylium chloride and its 4,6,3′-trimethyl derivative (I) which results in the formation of (1) and (2) (Scheme 1) (Jolibois, Vebrel, Ouahab, Boultif & Grandjean, 1988).



Scheme 1

The molecular structures consist of two associated flavane skeletons (I) and we deemed it necessary to determine precisely the junction points of this association. The inductive effect of supplementary methyl groups could induce a different type of linkage. We therefore determined the structures of compounds (1) and (2).

---

* Author to whom correspondence should be addressed.

0108-2701/89/091397-04$03.00

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å²)

$$B_{eq} = \tfrac{4}{3}\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Compound (1)				
O1	−0·0199 (2)	0·1641 (2)	0·3307 (1)	3·17 (5)
O2	0·3360 (2)	0·3598 (2)	0·2037 (1)	3·36 (5)
O3	0·3505 (2)	0·4184 (2)	0·3581 (1)	3·28 (5)
O4	0·1442 (2)	0·5686 (2)	0·3468 (2)	4·92 (6)
O5	−0·0012 (3)	0·7242 (3)	0·3806 (2)	8·08 (8)
C1	−0·1598 (3)	0·1555 (3)	0·2770 (2)	3·25 (7)
C2	−0·2521 (3)	0·1626 (3)	0·3293 (3)	4·47 (9)
C3	−0·3950 (4)	0·1567 (4)	0·2800 (3)	5·2 (1)
C4	−0·4425 (3)	0·1427 (3)	0·1804 (3)	5·1 (1)
C5	−0·3503 (3)	0·1354 (3)	0·1278 (3)	4·15 (9)
C6	−0·2047 (3)	0·1431 (3)	0·1748 (2)	3·29 (7)
C7	−0·0956 (3)	0·1417 (3)	0·1206 (2)	3·04 (7)
C8	0·0132 (3)	0·0869 (3)	0·1841 (2)	3·02 (7)
C9	0·0858 (3)	0·1887 (3)	0·2758 (2)	2·67 (6)
C10	0·2292 (3)	0·1841 (3)	0·3485 (2)	2·79 (6)
C11	0·2259 (2)	0·0680 (3)	0·3823 (2)	3·58 (7)
C12	0·3475 (4)	0·0675 (3)	0·4569 (3)	4·19 (8)
C13	0·4648 (3)	0·1837 (3)	0·4981 (3)	4·19 (8)
C14	0·4673 (3)	0·3008 (3)	0·4647 (2)	3·64 (8)
C15	0·3454 (3)	0·2991 (3)	0·3888 (2)	2·94 (7)
C16	0·2657 (3)	0·4128 (3)	0·2596 (2)	2·84 (7)
C17	0·1045 (3)	0·3217 (2)	0·2373 (2)	2·58 (6)
C18	0·0123 (3)	0·2899 (3)	0·1256 (2)	2·85 (7)
C19	0·1137 (3)	0·3014 (3)	0·0626 (2)	3·17 (7)
C20	0·2649 (3)	0·3320 (3)	0·1031 (2)	3·27 (7)
C21	0·3567 (3)	0·3399 (3)	0·0453 (3)	4·47 (8)
C22	0·2978 (4)	0·3210 (4)	−0·0541 (3)	5·29 (9)
C23	0·1473 (4)	0·2952 (4)	−0·0976 (2)	5·0 (1)
C24	0·0584 (4)	0·2859 (3)	−0·0397 (2)	4·25 (8)
C25	0·2905 (3)	0·5554 (3)	0·2458 (2)	3·15 (7)
C26	0·3832 (4)	0·6220 (3)	0·1934 (3)	4·26 (9)
C27	0·4077 (4)	0·7510 (3)	0·1800 (3)	5·3 (1)
C28	0·3389 (4)	0·8167 (3)	0·2196 (3)	4·8 (1)
C29	0·2478 (4)	0·7542 (3)	0·2726 (3)	4·12 (8)
C30	0·2255 (3)	0·6257 (3)	0·2882 (2)	3·46 (7)
C31	−0·1752 (4)	0·0606 (3)	0·0187 (2)	4·16 (9)
C32	−0·0711 (3)	0·3830 (3)	0·0973 (2)	3·51 (7)
C33	−0·1192 (5)	0·6966 (5)	0·3915 (3)	6·6 (1)
C34	−0·1870 (5)	0·7975 (6)	0·3888 (4)	9·9 (2)
C35	−0·1932 (8)	0·5715 (8)	0·4150 (7)	16·2 (3)
Compound (2)				
O1	0·2586 (2)	0·2458 (1)	0·5354 (1)	3·08 (5)
O2	0·4667 (2)	0·2428 (1)	0·8033 (1)	3·20 (5)
O3	0·5300 (2)	0·3070 (1)	0·7083 (1)	3·31 (5)
O4	0·6613 (2)	0·2177 (2)	0·6059 (1)	5·11 (7)
O5	0·7782 (3)	0·3314 (2)	0·9858 (2)	6·05 (7)
O6	0·7460 (2)	0·3899 (1)	0·8683 (2)	4·74 (6)
C1	0·2377 (3)	0·1838 (2)	0·4967 (2)	2·96 (7)
C2	0·2325 (3)	0·1821 (2)	0·4120 (2)	3·42 (8)
C3	0·2206 (3)	0·1214 (2)	0·3700 (2)	3·68 (8)
C4	0·2115 (3)	0·0609 (2)	0·4116 (2)	3·30 (8)
C5	0·2107 (3)	0·0651 (2)	0·4956 (2)	3·25 (7)
C6	0·2288 (3)	0·1251 (2)	0·5401 (2)	2·71 (7)
C7	0·2254 (3)	0·1298 (2)	0·6330 (2)	2·87 (7)
C8	0·1808 (3)	0·2006 (2)	0·6497 (2)	2·90 (7)
C9	0·2873 (3)	0·2433 (2)	0·6268 (2)	2·74 (7)
C10	0·2962 (3)	0·3163 (2)	0·6510 (2)	2·85 (7)
C11	0·1880 (3)	0·3588 (2)	0·6317 (2)	3·39 (8)
C12	0·1974 (4)	0·4278 (2)	0·6433 (2)	3·91 (8)
C13	0·3223 (4)	0·4547 (2)	0·6755 (2)	4·17 (9)
C14	0·4310 (3)	0·4136 (2)	0·6981 (2)	3·67 (8)
C15	0·4176 (3)	0·3448 (2)	0·6863 (2)	3·02 (7)
C16	0·5147 (3)	0·2385 (2)	0·7289 (2)	2·97 (7)
C17	0·4152 (3)	0·2025 (2)	0·6598 (2)	2·68 (7)
C18	0·3736 (3)	0·1311 (2)	0·6856 (2)	2·65 (7)
C19	0·3856 (3)	0·1276 (2)	0·7796 (2)	3·04 (7)
C20	0·4285 (3)	0·1820 (2)	0·8322 (2)	3·05 (7)
C21	0·4354 (4)	0·1792 (2)	0·0170 (2)	3·97 (8)
C22	0·3986 (4)	0·1212 (2)	0·9512 (2)	4·46 (9)
C23	0·3590 (3)	0·0646 (2)	0·9026 (2)	4·17 (9)
C24	0·3553 (3)	0·0689 (2)	0·8177 (2)	3·52 (8)
C25	0·6528 (3)	0·2101 (2)	0·7488 (2)	3·10 (7)
C26	0·7204 (3)	0·1986 (2)	0·8315 (2)	3·80 (8)
C27	0·8497 (4)	0·1759 (2)	0·8532 (2)	4·57 (9)
C28	0·9124 (4)	0·1673 (2)	0·7902 (3)	5·2 (1)
C29	0·8495 (3)	0·1801 (2)	0·7078 (2)	4·71 (9)
C30	0·7210 (3)	0·2023 (2)	0·6861 (2)	3·88 (8)
C31	0·1372 (3)	0·0759 (2)	0·6556 (2)	3·56 (8)
C32	0·4575 (3)	0·0753 (3)	0·6615 (2)	3·28 (7)
C33	0·2019 (4)	−0·0052 (2)	0·3672 (2)	4·62 (9)
C34	0·0800 (5)	0·4227 (2)	0·6205 (3)	5·7 (1)
C35	0·3193 (4)	0·0004 (2)	0·9391 (3)	5·9 (1)
C36	0·9194 (4)	0·1650 (3)	0·9438 (3)	6·6 (1)
C37	0·5735 (4)	0·3873 (2)	0·9338 (3)	5·5 (1)
C38	0·7089 (4)	0·3666 (2)	0·9334 (2)	4·37 (9)
C39	0·8703 (4)	0·3678 (2)	0·8561 (3)	5·3 (1)
C40	0·8700 (4)	0·3796 (2)	0·7673 (3)	5·8 (1)

Experimental. White parallelepiped crystals were grown by slow evaporation of an acetone (1) and an ethyl acetate (2) solution and were each sealed in a glass capillary; Nonius CAD-4 four-circle diffractometer, graphite-crystal-monochromatized Mo $K\alpha$ radiation. Cell dimensions: least-squares refinement on setting angles of 25 accurately centered reflections ($\theta \leq 12°$). Intensities collected by θ–2θ scans. Three standard reflections measured every hour: no fluctuation in intensity. Lorentz and polarization corrections, no absorption correction. Direct methods (*MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Full-matrix least-squares anisotropic (β_{ij}) refinement (H atoms placed in reasonable positions, isotropic, not refined), $\sum w(|F_o| - |F_c|)^2$ minimized, $w = [\sigma(|F_o|)^2 + (P.F_o)^2]^{-1}$. Scattering factors from *International Tables for X-ray Crystallography* (1974). All computing programs from Enraf–Nonius *SDP* described by Frenz (1978).

(1): Crystal dimensions: 0·45 × 0·27 × 0·12 mm; 4995 reflections collected with $2\theta \leq 50°$, $-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $0 \leq l \leq 16$, 2828 independent reflections with $I \geq 3\sigma(I)$, 362 parameters, $R = 0{\cdot}054$; $wR = 0{\cdot}074$, $P = 0{\cdot}07$, $S = 1{\cdot}73$, $(\Delta/\sigma)_{\max} = 0{\cdot}05$, $\Delta\rho_{\max} = 0{\cdot}30$ e Å^{-3}.

(2): Crystal dimensions: 0·45 × 0·27 × 0·12 mm; 3929 reflections collected with $2\theta \leq 50°$, $-12 \leq h \leq 12$, $0 \leq k \leq 23$, $0 \leq l \leq 19$, 2994 independent reflections with $I \geq 3\sigma(I)$, 416 parameters, $R = 0{\cdot}050$; $wR = 0{\cdot}070$, $P = 0{\cdot}07$, $S = 1{\cdot}60$, $(\Delta/\sigma)_{\max} = 0{\cdot}05$, $\Delta\rho_{\max} = 0{\cdot}23$ e Å^{-3}.

Atomic coordinates and equivalent isotropic thermal parameters are given in Table 1.*

Discussion. Selected bond lengths and bond angles are given in Table 2. The molecular structures and atom-numbering schemes are presented in Fig. 1. The geometrical parameters of the benzo and phenyl rings are in good agreement with those reported for compound (I) (Jolibois, Théobald, Vebrel, Laarif &

---

* Complete tables of bond distances and bond angles, lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51936 (57 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Selected bond distances* (Å) *and bond angles* (°), *with e.s.d.'s in parentheses*

	(1)	(2)
O3—C15	1·385 (4)	1·374 (4)
O3—C16	1·428 (3)	1·422 (4)
C7—C6	1·524 (5)	1·527 (4)
C7—C8	1·532 (4)	1·531 (5)
C7—C18	1·594 (4)	1·586 (4)
C7—C31	1·535 (4)	1·525 (5)
C9—O1	1·458 (4)	1·457 (4)
C9—C8	1·526 (4)	1·530 (5)
C9—C10	1·505 (4)	1·502 (5)
C9—C17	1·546 (4)	1·552 (4)
C17—C16	1·516 (3)	1·520 (4)
C17—C18	1·577 (4)	1·574 (4)
C18—C19	1·527 (5)	1·522 (4)
C18—C32	1·536 (5)	1·532 (5)
C15—O3—C16	116·2 (2)	116·4 (2)
C6—C7—C8	107·1 (3)	108·0 (2)
C6—C7—C18	107·9 (3)	108·0 (3)
C6—C7—C31	111·9 (2)	110·3 (2)
C8—C7—C18	100·8 (2)	101·1 (2)
C8—C7—C31	111·7 (3)	111·7 (3)
C18—C7—C8	116·5 (3)	117·2 (2)
O1—C9—C31	107·5 (2)	107·3 (2)
O1—C9—C10	103·3 (2)	102·9 (2)
O1—C9—C17	108·6 (3)	108·4 (3)
C8—C9—C10	117·4 (3)	118·2 (3)
C8—C9—C17	104·4 (2)	104·6 (3)
C10—C9—C17	115·3 (2)	115·0 (2)
C9—C17—C16	113·2 (2)	113·1 (3)
C9—C17—C18	107·2 (2)	106·8 (2)
C16—C17—C18	114·4 (2)	114·2 (2)
C7—C18—C17	100·1 (2)	99·9 (2)
C7—C18—C19	112·2 (3)	111·9 (3)
C7—C18—C32	113·2 (2)	113·7 (2)
C17—C18—C19	110·8 (2)	110·9 (2)
C17—C18—C32	111·3 (3)	111·4 (3)
C19—C18—C32	108·9 (3)	108·8 (2)

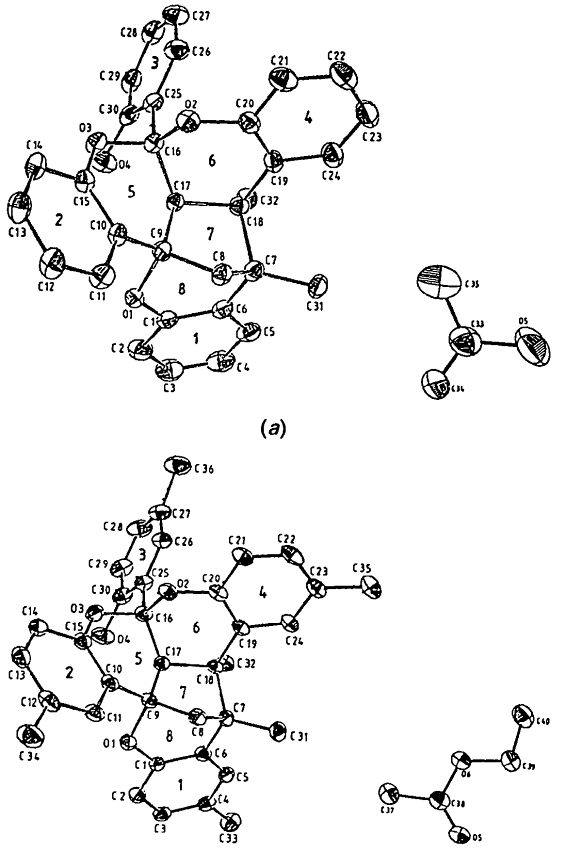
Table 3. *Comparison of certain bond distances* (Å) *and charges of trihydroxyflavylium,* (I), (1) *and* (2)

	(1)	(2)	(I)	Trihydroxy-flavylium
O1—C1	1·387 (4)*	1·383 (4)*	1·368 (4)	1·363 (6)
O1—C9	1·442 (4)*	1·439 (4)*	1·335 (4)	1·344 (6)
C16—C25	1·525 (4)	1·521 (4)	1·448 (4)	1·452 (4)
Charges	0	0	+	+

*Mean distances of the corresponding O—C bonds in the pyrano rings.

Devin, 1986) and 6,7,4′-trihydroxyflavylium chloride (Ueno & Saito, 1977), while the O—C (in the pyrano rings) and the C16—C25 bond lengths are longer (see Table 3).

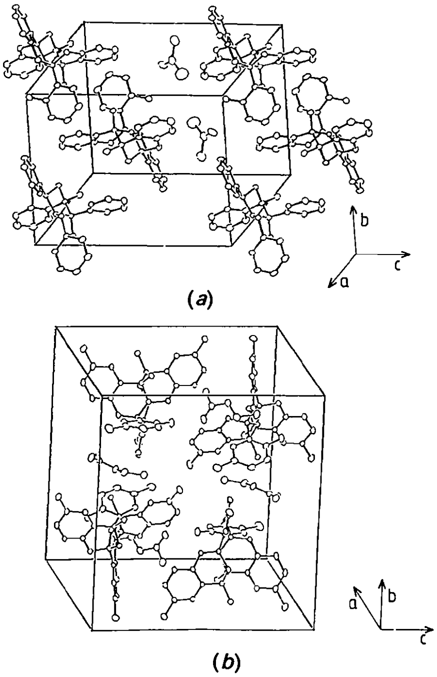
The molecular structures differ only in the number of methyl groups: two in (1), and six in (2). These structures can be described as an association of two flavane skeletons (I). This association is established *via* (i) the C atoms in position 4 of each fragment (C7···C18); (ii) the C atom in position 2 of the first fragment and the C atom in position 3 of the second (C9···C17); (iii) the hydroxyl O atom of the first fragment and the C atom in position 2 of the other (O3···C16) (see Scheme 1 for the atom positions). The association results in the formation of a five-membered ring 7 and a heterocycle 5. The benzo 1, 2 and 4, and the phenyl 3 rings are planar, while the pyrano rings 5, 6 and 8, and the five-membered ring 7 are not planar. The latter is the consequence of sp^3



(*a*)

(*b*)

Fig. 1. Views of the molecular structures showing atom numbering (*a*) of (1) and (*b*) of (2).



(*a*)

(*b*)

Fig. 2. Content of the unit cells (*a*) of (1) and (*b*) of (2).

hybridization of the C atoms concerned, by the junction, as indicated by the bond lengths and the bond angles around each.

Views of the unit cells are presented in Fig. 2. Short O4···O5 intermolecular distances of 2·726 (4) Å in (1) and 2·756 (4) Å in (2) are observed, indicating hydrogen bonding between the solvent molecules and the dimers.

References

FRENZ, B. A. (1978). *The Enraf–Nonius CAD-4 Structure Determination Package. A Real Time System for Concurrent X-ray Data Collection and Crystal Structure Solution*. In *Computing in Crystallography*, edited by H. SCHENK, R. OLTHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, pp. 64–71. Delft Univ. Press.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

JOLIBOIS, H., THÉOBALD, F., VEBREL, J., LAARIF, A. & DEVIN, C. (1986). *J. Chem. Res. (S)*, p. 56.

JOLIBOIS, H., VEBREL, J., OUAHAB, L., BOULTIF, A. & GRANDJEAN, D. (1988). *Helv. Chim. Acta*, **71**, 254–256.

JURD, L. & ROITMAN, J. N. (1978). *Tetrahedron*, **34**, 57–62.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

REYNOLDS, G. A. & VAN ALLAN, J. A. (1967). *J. Org. Chem.* **34**, 3616–3618.

REYNOLDS, G. A., VAN ALLAN, J. A. & REGAN, T. H. (1967). *J. Org. Chem.* **32**, 3772–3774.

UENO, K. & SAITO, N. (1977). *Acta Cryst.* B**33**, 111–113.

Acta Cryst. (1989). C**45**, 1400–1403

Structures of 2,2′,2″-Trimethoxytriphenylamine and 2,2′,2″-Trihydroxytriphenylammonium Benzenesulfonate

BY EDGAR MÜLLER*†

Laboratorium für anorganische Chemie, Swiss Federal Institute of Technology (ETH),
8092 Zürich, Switzerland

AND HANS-BEAT BÜRGI

Labor für chemische und mineralogische Kristallographie, Universität Bern, Freiestrasse 3,
3012 Bern, Switzerland

(*Received* 5 *October* 1988; *accepted* 23 *January* 1989)

Abstract. 2,2′,2″-Trimethoxytriphenylamine, (I): $C_{21}H_{21}NO_3$, M_r = 335·43, cubic, $Pa3$, a = 15·4265 (10) Å, V = 3671·2 Å^3, Z = 8, D_x = 1·214 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 0·756 cm^{-1}, F(000) = 1424, T = 295 K, R = 0·037 for 582 observed reflections ($> \sigma_F$) and 104 parameters. 2,2′,2″-Trihydroxytriphenylammonium benzenesulfonate, (II): $C_{18}H_{16}NO_3^+.C_6H_5O_3S^-$, M_r = 451·497, monoclinic, $P2_1/c$, a = 9·654 (3), b = 10·686 (3), c = 21·019 (5) Å, β = 95·18 (1)°, V = 2159·5 Å^3, Z = 4, D_x = 1·389 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 1·820 cm^{-1}, F(000) = 944, T = 295 K, R = 0·058 for 2082 observed reflections ($> \sigma_F$) and 374 parameters. Both compounds adopt a propellerlike conformation with a crystallographic and local C_3 axis respectively. The C—O distances in (I) and (II), as well as the C—N distances in (I), are shorter than the sum of the corresponding covalent single-bond radii, due to conjugation of the O and N lone pairs with the aromatic rings. The environment of the N atom in (I) is almost planar. Protonation pyramidalizes the geometry of the N atom [in (II)], and the C—N distances elongate towards the corresponding single-bond values.

Introduction. The structure determinations of the title compounds were part of a larger study on complexes of 2,2′,2″-trihydroxytriphenylamine (= 2,2′,2″-nitrilotriphenole = H_3NTPH) (Müller, 1982; Müller & Bürgi, 1987). The structures presented here serve as reference data for the interpretation of observed structural variations within the NTPH skeleton upon formation of complexes.

Experimental. 2,2′,2″-Trimethoxytriphenylamine [(I), Me_3NTPH] and 2,2′,2″-trihydroxytriphenylamine (H_3NTPH) were obtained as described by Frye, Vincent & Hauschildt (1966). 2,2′,2″-Trihydroxytriphenylammonium benzenesulfonate (II) was obtained from H_3NTPH and benzenesulfonic acid in

---

* Author to whom correspondence should be addressed.

† Currently at Leiden University, Department of Chemistry (Gorlaeus Laboratories), Einsteinweg 5, 2300 RA Leiden, The Netherlands.

0108-2701/89/091400-04$03.00