C(43)—C(42)—C(46)	108.2 (10)	C(51)—C(56)—C(55)	120.8 (11)
C(43)—C(44)—C(45)	100.3 (10)	C(52)—C(51)—C(56)	118.0 (11)
C(44)—C(45)—C(46)	106.8 (9)	C(52)—C(53)—C(54)	121.2 (13)
C(44)—C(45)—C(49)	114.7 (10)	C(53)—C(54)—C(55)	119.3 (14)
C(45)—C(41)—C(47)	89.6 (8)	C(54)—C(55)—C(56)	121.8 (13)

Data were corrected for Lorentz and polarization effects. The structure was solved by direct methods using *SHELXTL-Plus* (Sheldrick, 1989). Blocked least-squares refinements were carried out with *SHELX*76 (Sheldrick, 1976). Anisotropic refinement reduced *R* to 0.094. H atoms were added at idealized positions and included in the final refinement.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HL1036). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Molecules Isoelectronic with 2,2,2-Triphenylethanol: Multiple Hydrogen-Bonding Modes in the Structures of *O*-Tritylhydroxylamine, Ph_3CONH_2, and Triphenylmethanesulfenamide, Ph_3CSNH_2

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Abstract

O-Tritylhydroxylamine, $C_{19}H_{17}NO$ (IV), forms dimers in the solid state which are made up from two different molecules; these dimers exhibit three type of hydrogen bond, intermolecular N—H···N and N—H···π(arene), and intramolecular (aryl)C—H···O. Triphenylmethanesulfenamide, $C_{19}H_{17}NS$ (V), forms centrosymmetric dimers in the solid state in which N—H···S hydrogen bonds are the sole type observed.

Comment

Some general principles underlying hydrogen-bond formation in systems containing equal numbers of hydrogen-bond donors and acceptors have been formulated recently (Etter, 1990; Etter, MacDonald & Bernstein, 1990). The strongest hydrogen-bond donor will interact preferentially with the strongest acceptor, followed by the next-strongest donor and acceptor pair and so on until all the hydrogen-bond donor and acceptor capacity has been employed. Where there is a numerical mismatch between hydrogen-bond donors and acceptors, an excess of donors can often be accommodated either by formation of *X*—H···π(arene) hydrogen bonds or by a change of hybridization at the acceptor site (Hanton, Hunter & Purvis, 1992), while an excess of acceptors can be accommodated by formation of C—H···*X* hydrogen bonds involving C—H bonds on benzenoid rings as hydrogen-bond donors (Hunter, 1991).

We have recently tested these general ideas by comparing the hydrogen bonding in three isoelectronic and isosteric molecular systems, Ph_3COH (I), Ph_3CNH_2 (II) and $Ph_2C(C_5H_4N)OH$ (III). In this series, (I) contains equal numbers of hydrogen-bond donors and acceptors, (II) contains an excess of donors and (III) contains an excess of acceptors. It is found that whereas compound (I) forms tetrahedral tetrameric hydrogen-bonded aggregates (Ferguson, Gallagher, Glidewell, Low & Scrimgeour, 1992), (II) forms no hydrogen bonds at all (Glidewell & Ferguson, 1994), and of the potential hydrogen-bond acceptor sites in (III), only the N atom is used and the O atom is not involved in any hydrogen bonding at all (Glidewell & Ferguson, 1994).

As a further test, we have now compared the structures of *O*-tritylhydroxylamine, Ph_3CONH_2 (IV), and triphenylmethanesulfenamide, Ph_3CSNH_2 (V), with the isosteric 2,2,2-triphenylethanol, Ph_3CCH_2OH (VI) (Ferguson, Glidewell & Zakaria, 1994). Both (IV) and (V) contain two potential hydrogen-bond donors (in the NH_2 groups) and two potential acceptor sites (N and O or S) per molecule, but compound (VI) contains just one donor and one acceptor per molecule. Hence the numbers of hydrogen-bond donors and acceptors in each compound are matched, although their identities differ. The structure of (VI) consists of cyclic, almost planar centrosymmetric tetramers built up using only O—H···O hydrogen bonds with precise pairing of donors and acceptors (Ferguson, Glidewell & Zakaria, 1994). Compound (IV), by contrast, crystallizes as dimers in which the principal intermolecular hydrogen bonding is of the N—H···N type with the O atoms, unused in in-

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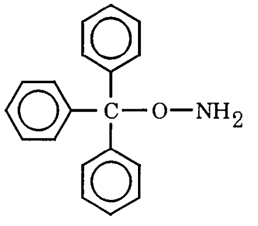
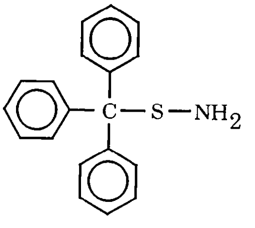
termolecular hydrogen bonding, forming intramolecular C—H···O bonds and with one of the N—H bonds forming intermolecular N—H···π(arene) hydrogen bonds. Compound (V) also forms dimers, where the only hydrogen bonds are of the N—H···S type.



(IV)



(V)

O-Tritylhydroxylamine (IV) crystallizes with two independent molecules in the asymmetric unit (labelled *A* and *B* in Fig. 1). These two molecules are linked into a dimeric aggregate by N—H···N hydrogen bonds in a motif of graph set $R^2_2(4)$ (Etter, 1990; Etter, MacDonald & Bernstein, 1990); the N···N distance is 3.228 (4) and the NH···N distances are 2.62 and 2.94 Å giving a very asymmetric hydrogen-bonded ring. Formation of this ring employs one hydrogen-bond donor and one acceptor per molecule, leaving free one N—H donor and the O atom as acceptor in each molecule; in addition to these intermolecular hydrogen bonds, there are also intramolecular hydrogen bonds. The C12—H12 bond acts as hydrogen-bond donor to oxygen in both molecules *A* and *B* in a motif of graph set $S(5)$; the CH···O distances are 2.29 and 2.25 Å, respectively, in molecules *A* and *B*. It would be tempting to associate these intramolecular bonds with the narrow O—C1—C11 bond angles which are 103.3 (2) and 103.6 (2)° in molecules *A* and *B*, respectively; however, a similar bond angle occurs in compound (V) without any such intramolecular hydrogen bonding. Finally, there are intermolecular N—H···π(arene) interactions involving both the N*B*—H*NB*1 bond in molecule *B* acting as hydrogen-bond donor and two aromatic ring C atoms (C25*A* and C26*A*) in molecule *A* acting as acceptor, and the hitherto unused N*B*—H*NB*2 bond acting as donor to C22*A*; the H···C distances are 2.87, 2.73 and 2.85 Å, respectively, all well within the sum of the van der Waals radii. The H atom H*NA*1 appears to take part in no hydrogen bonds. Overall, however, the hydrogen-bonding scheme exhibits two of the important types of interaction [*X*—H···π(arene) and aromatic C—H···*X*] expected when 'conventional' *X*—H···*Y* hydrogen bonding cannot accommodate all the potential hydrogen-bonding capacity of a system (Hunter, 1991; Hanton, Hunter & Purvis, 1992).

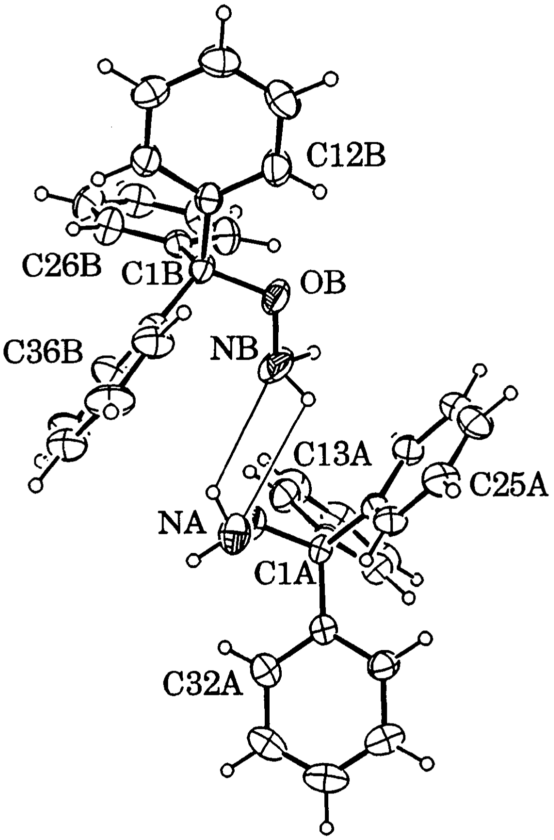


Fig. 1. View of the hydrogen-bonded dimer of Ph_3CONH_2 (IV) with atomic numbering scheme indicated. The non-H atoms are shown as displacement ellipsoids drawn at the 30% probability level. For clarity, H atoms are drawn as small spheres of arbitrary size

Within the molecules of (IV), the C1—C*n*1 bonds [*n* = 1, 2, 3; mean 1.532 (2) Å] are all well above the upper quartile value of 1.521 Å for $C(sp^3)$—C(aryl) bonds (Allen *et al.*, 1987), but still shorter than the mean value of 1.543 (2) Å found in compound (VI) (Ferguson, Glidewell & Zakaria, 1994). The mean of the 36 phenyl C—C distances in molecules *A* and *B* is 1.375 (11) Å. The C—O bond lengths are entirely typical of bonds of type R_3C—O*X*. Similarly, the O—N distances are typical of such bonds in cases where the N atoms are pyramidal, as found here – much shorter bonds are observed with planar N atoms. The pyramidal nature of the N atoms is demonstrated both by the sum of interbond angles (299 and 301°) and by their behaviour as hydrogen-bond acceptors. The principal differences between molecules *A* and *B* in compound (IV) are in the orientations of the phenyl rings.

Triphenylmethanesulfenamide (V) crystallizes as centrosymmetric dimers held together by N—H···S hydrogen bonds (Fig. 2) in a motif with graph set $R^2_2(6)$; the S···N and S···H distances are 3.601 (2) and 2.82 Å, respectively. The N atom takes part in neither inter- nor intramolecular hydrogen bonds. The short intramolecular S···H contacts involving H12, H22 and H32 (at distances of 2.79, 2.67 and 2.88 Å, respectively) are all within the sum of the van der Waals radii, but probably depend in part on the concerted twist of the three phenyl rings, whose S—C1—C*n*1—C*n*2 torsion angles

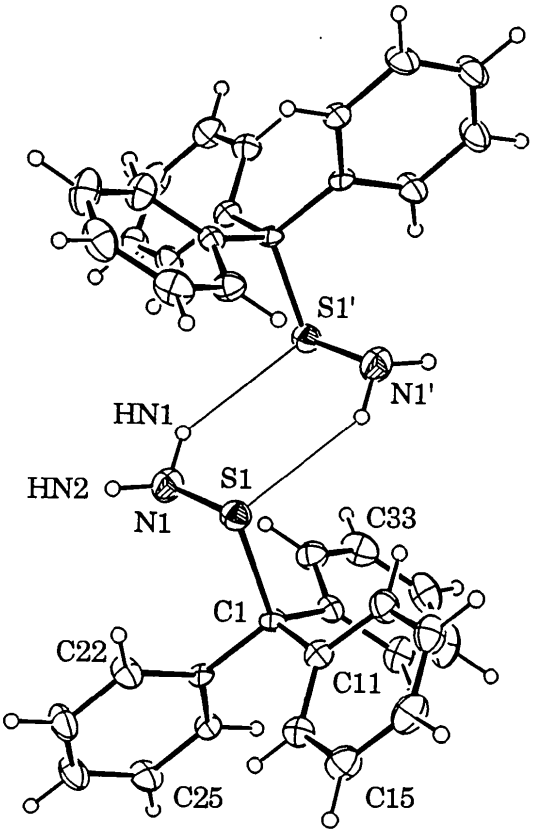


Fig. 2. The centrosymmetric hydrogen-bonded dimer of Ph_3CSNH_2 (V) with atomic numbering scheme. The non-H atoms are shown as displacement ellipsoids drawn at the 30% probability level. For clarity, H atoms are drawn as small spheres of arbitrary size

are −57.7 (3), −33.9 (2) and −46.4 (3)° for $n = 1$, 2 and 3, respectively. These contacts cannot all represent genuine hydrogen bonds because sulfur has insufficient lone pairs and it is noteworthy that the small S—C1—C11 angle of 99.8 (1)° is not associated with the shortest of the S···*HC* contacts.

The C1—C*n*1 bonds in (V) have a mean value of 1.535 (2) Å, very similar to that found in (IV), and the mean of the 18 phenyl C—C distances is 1.383 (9) Å. The C—S distance, 1.873 (2) Å, is typical of its type (Allen *et al.*, 1987). The S—N distance of 1.698 (2) Å on the other hand is much closer to the values characteristic of *R*S—NX_2 bonds involving planar N atoms [mean value 1.707 (19) Å] than to examples involving pyramidal N atoms [1.765 (3) Å] (Auricchio, Brückner, Malpezzi Giunchi, Kozinsky & Zelenskaja, 1980). Consistent with this, the pyramidal character of the N atom in (V) is much less marked than in (IV), the sum of the interbond angles at the N atom being 325° compared with 300° in (IV). In terms of Etter's (1990) rules for hydrogen-bond formation, it may be inferred that in compound (IV), the N atom is a stronger hydrogen-bond acceptor than the O atom, while in compound (V) the S atom is a better acceptor than the N atom. The enhanced basicity of sulfur in (V) (associated with the short S—N bond), the less pyramidal N atom, and the conformation of the NH_2 group (C1—S—N—H torsion angles of 116 and −125°) are all consistent with, although not evidence for, some intramolecular *pπ–dπ* interaction between the N and S atoms. Hence in this instance the third strategy for dealing with donor/acceptor mismatch, a change in hybridization at the N acceptor site (Hanton, Hunter & Purvis, 1992), appears to have occurred. The changes in hydrogen-bonding behaviour observed in the series (IV), (V) and (VI) are thus consistent with the mismatch strategies postulated by Hunter and his colleagues whereas the closely related pair (I) and (II) show behaviour wholly inconsistent with these strategies.

Experimental

Crystals of Ph_3CONH_2 (IV) and Ph_3CSNH_2 (V) were grown from solution in methanol and dichloromethane/light petroleum (b.p. 313–333 K), respectively; the starting materials are commercially available (Aldrich). Crystals of Ph_3CONH_2 grown from dichloromethane/light petroleum proved to have cell dimensions identical to those of the sample grown from methanol.

Compound (IV)

Crystal data

$C_{19}H_{17}NO$
$M_r = 275.35$
Triclinic
$P\bar{1}$
$a = 8.8763$ (19) Å
$b = 12.343$ (2) Å
$c = 15.033$ (3) Å
$\alpha = 68.708$ (14)°
$\beta = 85.38$ (3)°
$\gamma = 77.50$ (3)°
$V = 1498.3$ (5) Å^3
$Z = 4$
$D_x = 1.221$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 9.50$–17.50°
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Needle
0.40 × 0.15 × 0.15 mm
Colourless

Data collection

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
6513 measured reflections
6513 independent reflections
2907 observed reflections (weak diffraction, only 44.6% observed) [$I > 3.0\sigma(I)$]

$\theta_{\max} = 26.90°$
$h = -11 \rightarrow 11$
$k = 0 \rightarrow 15$
$l = -19 \rightarrow 19$
3 standard reflections
frequency: 60 min
intensity variation: <1.0% variation, no decay

Refinement

Refinement on F
$R = 0.038$

Extinction correction: Larson (1970)

$wR = 0.051$
$S = 1.27$
2907 reflections
380 parameters
$w = 1/[\sigma^2(F) + 0.0008F^2]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}
Extinction coefficient: $5.4 (13) \times 10^3$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (IV)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
OA	0.57842 (19)	0.04395 (14)	0.08822 (12)	0.0600 (12)
NA	0.7113 (3)	−0.05390 (18)	0.11338 (18)	0.0761 (17)
C1A	0.6286 (3)	0.15657 (19)	0.05399 (16)	0.0446 (14)
C11A	0.4769 (3)	0.2483 (2)	0.02611 (16)	0.0456 (14)
C12A	0.3347 (3)	0.2193 (3)	0.0561 (2)	0.066 (2)
C13A	0.2004 (3)	0.3047 (4)	0.0295 (2)	0.082 (3)
C14A	0.2053 (4)	0.4186 (3)	−0.0262 (2)	0.079 (2)
C15A	0.3444 (4)	0.4494 (2)	−0.0547 (2)	0.072 (2)
C16A	0.4791 (3)	0.3649 (2)	−0.02887 (18)	0.0576 (16)
C21A	0.7108 (3)	0.16797 (19)	0.13488 (15)	0.0442 (14)
C22A	0.6337 (3)	0.2284 (2)	0.19196 (17)	0.0543 (16)
C23A	0.7062 (4)	0.2369 (2)	0.26649 (18)	0.068 (2)
C24A	0.8588 (4)	0.1840 (3)	0.28536 (19)	0.072 (2)
C25A	0.9374 (3)	0.1217 (3)	0.23058 (19)	0.0666 (19)
C26A	0.8646 (3)	0.1133 (2)	0.15639 (17)	0.0547 (16)
C31A	0.7264 (3)	0.16710 (19)	−0.03621 (16)	0.0460 (14)
C32A	0.6900 (3)	0.1187 (2)	−0.0999 (2)	0.0614 (18)
C33A	0.7708 (4)	0.1317 (3)	−0.1846 (2)	0.074 (2)
C34A	0.8890 (4)	0.1920 (3)	−0.2065 (2)	0.079 (2)
C35A	0.9254 (3)	0.2413 (3)	−0.1453 (2)	0.071 (2)
C36A	0.8437 (3)	0.2299 (2)	−0.06084 (17)	0.0575 (17)
OB	0.6757 (2)	−0.14104 (14)	0.43542 (12)	0.0641 (11)
NB	0.6543 (3)	−0.0780 (2)	0.33396 (16)	0.0885 (18)
C1B	0.6091 (3)	−0.24620 (19)	0.46553 (15)	0.0461 (14)
C11B	0.6585 (3)	−0.30999 (19)	0.57018 (16)	0.0440 (14)
C12B	0.7206 (3)	−0.2555 (2)	0.61924 (19)	0.0659 (18)
C13B	0.7621 (4)	−0.3146 (3)	0.7146 (2)	0.077 (2)
C14B	0.7408 (3)	−0.4266 (3)	0.76232 (18)	0.066 (2)
C15B	0.6792 (3)	−0.4814 (2)	0.71465 (18)	0.0656 (19)
C16B	0.6383 (3)	−0.4242 (2)	0.62007 (17)	0.0572 (17)
C21B	0.4326 (3)	−0.21146 (19)	0.46163 (15)	0.0446 (14)
C22B	0.3557 (3)	−0.0978 (2)	0.4518 (2)	0.066 (2)
C23B	0.1967 (4)	−0.0678 (3)	0.4477 (2)	0.080 (2)
C24B	0.1109 (3)	−0.1490 (3)	0.45510 (19)	0.069 (2)
C25B	0.1841 (3)	−0.2622 (3)	0.4680 (2)	0.072 (2)
C26B	0.3437 (3)	−0.2937 (2)	0.4714 (2)	0.0629 (18)
C31B	0.6778 (3)	−0.3200 (2)	0.40381 (16)	0.0471 (14)
C32B	0.8265 (3)	−0.3861 (3)	0.41985 (18)	0.0654 (19)
C33B	0.8947 (3)	−0.4481 (3)	0.3620 (2)	0.079 (2)
C34B	0.8163 (4)	−0.4461 (3)	0.2874 (2)	0.072 (2)
C35B	0.6714 (4)	−0.3790 (3)	0.2684 (2)	0.079 (2)
C36B	0.6021 (3)	−0.3163 (3)	0.32568 (19)	0.0679 (19)

Table 2. *Selected geometric parameters* (Å, °) *for* (IV)

OA—NA	1.455 (3)	OB—NB	1.445 (3)
OA—C1A	1.451 (3)	OB—C1B	1.450 (3)
NA—HNA1	0.92	NB—HNB1	0.92
NA—HNA2	0.89	NB—HNB2	1.06
C1A—C11A	1.535 (3)	C1B—C11B	1.533 (3)
C1A—C21A	1.531 (3)	C1B—C21B	1.532 (3)
C1A—C31A	1.530 (3)	C1B—C31B	1.531 (3)
NA—OA—C1A	110.19 (16)	OB—NB—HNB1	114
OA—NA—HNA1	101	OB—NB—HNB2	99
OA—NA—HNA2	102	HNB1—NB—HNB2	88
HNA1—NA—HNA2	96	OB—C1B—C11B	103.59 (16)
OA—C1A—C11A	103.30 (17)	OB—C1B—C21B	110.36 (18)
OA—C1A—C21A	109.15 (17)	OB—C1B—C31B	108.39 (18)
OA—C1A—C31A	109.61 (18)	C11B—C1B—C21B	108.58 (18)
C11A—C1A—C21A	111.81 (18)	C11B—C1B—C31B	111.91 (18)
C11A—C1A—C31A	108.31 (18)	C21B—C1B—C31B	113.56 (18)
C21A—C1A—C31A	114.10 (18)	NA—HNA2—NB	126
NB—OB—C1B	110.16 (16)	NB—HNB1—NA	100
C1A—OA—NA—HNA1	−123	C1B—OB—NB—HNB1	−143
C1A—OA—NA—HNA2	138	C1B—OB—NB—HNB2	126

Compound (V)

Crystal data

$C_{19}H_{17}NS$
$M_r = 291.41$
Triclinic
$P\overline{1}$
$a = 8.9918 (9)$ Å
$b = 8.9999 (11)$ Å
$c = 10.8780 (12)$ Å
$\alpha = 85.225 (9)°$
$\beta = 74.551 (8)°$
$\gamma = 63.082 (9)°$
$V = 755.85 (15)$ Å^3
$Z = 2$
$D_x = 1.280$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 18.00–23.50°$
$\mu = 0.20$ mm^{-1}
$T = 293$ K
Needle
$0.36 \times 0.22 \times 0.22$ mm
Pale yellow

Data collection

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
3277 measured reflections
3277 independent reflections
2548 observed reflections $[I > 3.0\sigma(I)]$
$\theta_{\max} = 26.89°$
$h = -9 \rightarrow 11$
$k = 0 \rightarrow 11$
$l = -13 \rightarrow 13$
3 standard reflections
frequency: 60 min
intensity variation: <1.0% variation, no decay

Refinement

Refinement on F
$R = 0.037$
$wR = 0.057$
$S = 1.58$
2548 reflections
190 parameters
$w = 1/[\sigma^2(F) + 0.0008F^2]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (V)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
S1	−0.01135 (6)	0.28418 (6)	0.02537 (4)	0.0404 (3)
N1	0.1898 (2)	0.2698 (2)	−0.00213 (17)	0.0530 (11)
C1	−0.0699 (2)	0.2439 (2)	0.19908 (16)	0.0315 (9)
C11	−0.2284 (2)	0.2170 (2)	0.20527 (16)	0.0336 (9)
C12	−0.3686 (2)	0.3424 (2)	0.16715 (19)	0.0418 (11)
C13	−0.5111 (3)	0.3209 (3)	0.1673 (2)	0.0503 (13)
C14	−0.5193 (3)	0.1742 (3)	0.2083 (2)	0.0537 (15)
C15	−0.3833 (3)	0.0506 (3)	0.2496 (2)	0.0503 (13)
C16	−0.2389 (3)	0.0707 (2)	0.24674 (19)	0.0419 (11)
C21	0.0784 (2)	0.0875 (2)	0.23136 (16)	0.0322 (10)
C22	0.1815 (3)	−0.0466 (2)	0.14392 (19)	0.0472 (12)
C23	0.3116 (3)	−0.1893 (3)	0.1757 (2)	0.0596 (15)
C24	0.3417 (3)	−0.2009 (3)	0.2941 (2)	0.0560 (14)
C25	0.2401 (3)	−0.0704 (3)	0.3820 (2)	0.0501 (13)
C26	0.1094 (2)	0.0731 (2)	0.35095 (17)	0.0385 (10)
C31	−0.1182 (2)	0.39522 (19)	0.28451 (16)	0.0334 (9)
C32	−0.0170 (3)	0.4789 (2)	0.26180 (19)	0.0453 (12)
C33	−0.0574 (3)	0.6122 (3)	0.3419 (2)	0.0563 (15)

C34	−0.1977 (3)	0.6622 (3)	0.4451 (2)	0.0575 (14)
C35	−0.2964 (3)	0.5790 (3)	0.4707 (2)	0.0617 (16)
C36	−0.2579 (3)	0.4461 (3)	0.3908 (2)	0.0488 (13)

Table 4. *Selected geometric parameters* (Å, °) *for* (V)

S1—N1	1.6980 (18)	C1—C11	1.534 (2)
S1—C1	1.8729 (17)	C1—C21	1.533 (2)
N1—H*N*1	0.88	C1—C31	1.538 (2)
N1—H*N*2	0.91		
N1—S1—C1	104.49 (8)	S1—C1—C31	111.91 (11)
S1—N1—H*N*1	106	C11—C1—C21	112.44 (13)
S1—N1—H*N*2	107	C11—C1—C31	111.13 (13)
H*N*1—N1—H*N*2	112	C21—C1—C31	111.14 (13)
S1—C1—C11	99.82 (11)	N1—S1—H*N*1^{i}	96
S1—C1—C21	109.92 (11)		
C1—S1—N1—H*N*1	−125	C1—S1—N1—H*N*2	116

Symmetry code: (i) $-x, 1-y, -z$.

Both (IV) and (V) crystallized in the triclinic system; space group $P\bar{1}$ was assumed and confirmed by the succesful refinement. All H atoms bonded to C atoms were clearly visible in difference maps; they were positioned geometrically (C—H 0.95 Å) and included as riding atoms in the structure-factor calculations. The coordinates of the H atoms bonded to the N atoms were obtained from difference maps and included but not refined in the calculations. Electron-density sections showing the H atoms bonded to the N atoms have been deposited. Examination of the structures with *PLATON* (Spek, 1992) showed that there were no solvent-accessible voids in the crystal lattices. Data collection and cell refinement: *CAD*-4 *Software* (Enraf-Nonius, 1989). Data reduction, structure solution and refinement, preparation of material for publication: *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). Figs. 1 and 2 were prepared using *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, along with electron-density sections showing the H atoms bonded to the N atoms have been deposited with the IUCr (Reference: AB1184). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(2*S*,3*R*,4*S*,5*R*,6*S*,7*R*,8*R*,9*S*)-1,2,3,4,5,6,7,8,9-Nonaacetoxydecane

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Abstract

The structure of the title compound, $C_{28}H_{40}O_{18}$, has been determined by X-ray diffraction. The acetoxy groups are planar and are approximately perpendicular to the carbon backbone, which adopts a *gauche* conformation around the C3—C4 bond.

Comment

This work is part of a project concerning the stereoselective synthesis of long-chain polyols from tartrate derivatives (Marshall, Beaudoin & Lewinski, 1993). The chain C1 to C10 in the title compound (I) contains two regions of extended conformation, C1 to C4 and C3 to C10, in a *gauche* orientation to each other. The average C—C bond length in the chain is 1.523 (9) Å and the average C—C—C angle is 113.5 (15)°, in agreement with the values found in other structures, especially with the average values of 1.523 (8) Å and 113.2 (5)° found in hexadecyltrimethylammonium bromide (Campanelli & Scaramuzza, 1986). All nine acetoxy groups are planar (average r.m.s. deviation 0.004 Å) and adopt a typical conformation with the C═O bonds pointing in the same direction as the C—H bonds (Abboud, Simonsen, Voll & Younathan, 1990). The torsion angles C—O—C—H vary from 0.1 to 28.1°. The average bond distances in the acetoxy groups are C_{sp^3}—O 1.442 (9), O—C_{sp^2} 1.355 (6), C_{sp^2}—$C_{\rm methyl}$ 1.482 (10)

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