[Bis(2-hydroxyethyl)amino]tris(hydroxymethyl)-methane (Bis–Tris), an important complexing agent

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The title compound, $(HOCH_2CH_2)_2NC(CH_2OH)_3$ or $C_8H_{19}NO_5$, is an important complexing agent. All hydroxyl-H atoms are involved in intermolecular hydrogen bonds (O—H$\cdots$O distances are in the range 2.690–2.847 Å), which link the molecules in the crystal into a three-dimensional infinite network. One of the hydroxymethyl hydroxyl groups also participates in an intramolecular O—H$\cdots$N hydrogen bond, closing a five-membered N—C—C—O—H pseudo-cycle [O$\cdots$N 2.7804 (16) Å and O—H$\cdots$N 118.6 (17)°].

Comment

The title compound, (I), commonly called Bis–Tris, is an important polyalcohol used in the complexation of metal ions (Hong *et al.*, 1995; Sigel *et al.*, 1982; Scheller *et al.*, 1980; Wesolowski & Palmer, 1989; Wesolowski *et al.*, 1990). It has received special attention as a chelating agent for some lanthanide ions (Oh *et al.*, 1998; Chen *et al.*, 1997; Pfefferle & Bunzli, 1989). The structure of (I) was determined in the course of an ongoing investigation into the complexation properties of Bis–Tris with various lanthanide halides (Wood *et al.*, 2000).

(I)
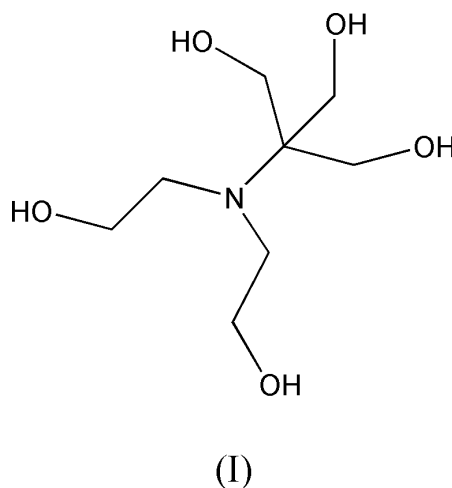
All five hydroxyl–H atoms in (I) (Fig. 1) are involved in intermolecular hydrogen bonds (Table 1), which link the molecules in the crystal of (I) into a three-dimensional infinite network. Fig. 2 shows the three-dimensional network down [010]. It can be seen from this direction that the hydrogen bonding is localized in regular supramolecular synthons (Desiraju & Steiner, 2001). One of these synthons is shown in Fig. 3 and Fig. 4.

The O3—H3 hydroxyl group also serves as a donor for an intramolecular O3—H3$\cdots$N1 bond (see Table 1), thus giving
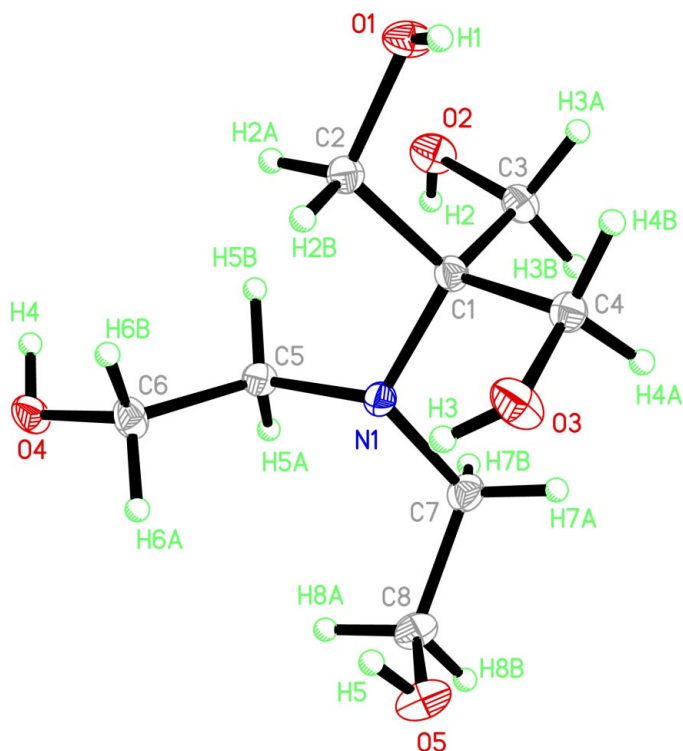
Figure 1
The molecular structure of (I) with atom labels and 30% probability ellipsoids for non-H atoms.

Figure 2
A view down [010] showing the extensive hydrogen bonding. Intermolecular interactions are indicated by dashed lines. Only H atoms involved in intermolecular interactions are shown.
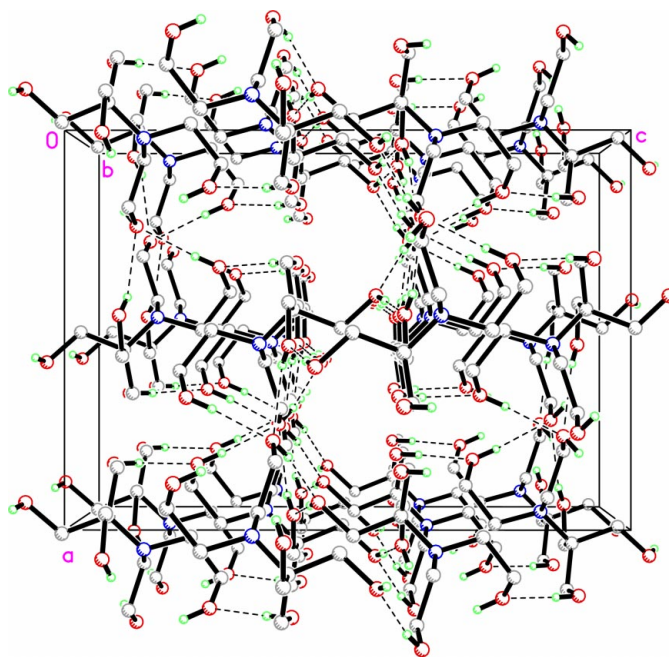
rise to a bifurcated hydrogen bond and closing the five-membered N1—C1—C4—O3—H3 pseudo-cycle. There are two other possibilities for intramolecular hydrogen bonding in (I). However, the C4—H4B···O1 and C5—H5B···O2 inter-actions should, in fact, be classified as extremely weak, if existing at all. As these are not bifurcated, it appears that this bonding is geometrically unlikely in the former, and extremely weak in the latter case. The corresponding distances and angles, are, nevertheless, included in Table 1 for comparison.

Experimental

The title compound was obtained commercially (Aldrich) and crystallized from a concentrated methanol solution.

Crystal data

$C_8H_{19}NO_5$	Mo $K\alpha$ radiation
$M_r = 209.24$	Cell parameters from 1001
Orthorhombic, $Pbca$	reflections
$a = 12.1298 (17)$ Å	$\theta = 2.4–27.9°$
$b = 9.5303 (13)$ Å	$\mu = 0.12$ mm^{-1}
$c = 17.144 (2)$ Å	$T = 203 (2)$ K
$V = 1981.9 (5)$ Å^3	Needle, colorless
$Z = 8$	$0.32 \times 0.20 \times 0.11$ mm
$D_x = 1.403$ Mg m^{-3}	

Data collection

Siemens SMART 1K	1745 independent reflections
diffractometer	1476 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.033$
Absorption correction: empirical	$\theta_{max} = 25.0°$
(*SADABS*; Sheldrick, 1999)	$h = -14 \rightarrow 11$
$T_{min} = 0.964$, $T_{max} = 0.987$	$k = -11 \rightarrow 11$
14160 measured reflections	$l = -20 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$+ 0.7334P]$
$wR(F^2) = 0.084$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
1745 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
147 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
H atoms treated by a mixture of	
independent and constrained	
refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^i	0.84 (2)	1.86 (2)	2.6897 (16)	177 (2)
O2—H2···O5^{ii}	0.81 (2)	2.03 (2)	2.8410 (17)	174 (2)
O3—H3···N1	0.78 (2)	2.321 (19)	2.7804 (16)	118.6 (17)
O3—H3···O4^{iii}	0.78 (2)	2.19 (2)	2.8466 (17)	141.6 (18)
O4—H4···O1^{iv}	0.81 (2)	1.99 (2)	2.7913 (16)	171 (2)
O5—H5···O4^{iii}	0.82 (2)	2.03 (2)	2.8251 (17)	165.6 (19)
C4—H4B···O1	0.98	2.57	2.9505 (18)	103
C5—H5B···O2	0.98	2.44	3.1192 (18)	126

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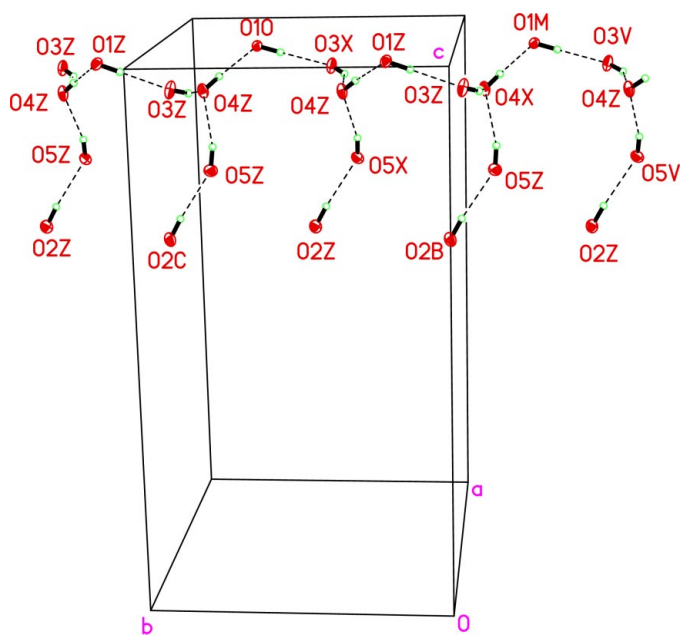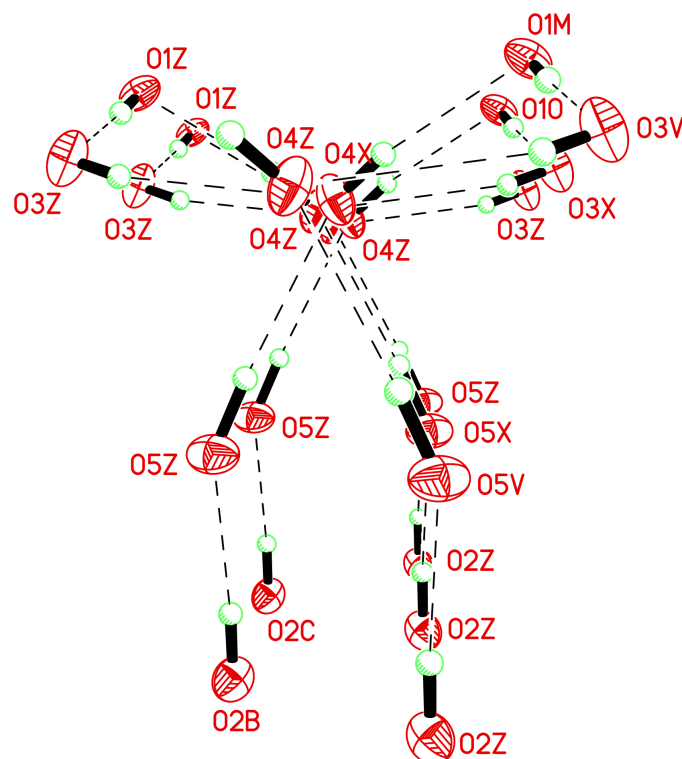
Figure 3

A view of the hydrogen-bonding synthon parallel to the [010] direction. Only O and H atoms involved in hydrogen bonding are shown. O atoms are shown with 30% probability ellipsoids.

Figure 4

The hydrogen-bonding synthon viewed down [010]. Only O and H atoms involved in hydrogen bonding are shown. O atoms are shown with 30% probability ellipsoids.

All hydroxyl-H atoms were located and refined (O—H 0.78–0.84 Å). All the rest of the H atoms were placed geometrically and included in the refinement in the riding-motion approximation with displacement parameters equal to $1.2U_{eq}$ of the corresponding carrier atom.

Data collection: *SMART* (Bruker, 1997–1998); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1999); program(s) used to solve structure: *XS* in *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *XL* in *SHELXTL*; molecular graphics: *XP* in *SHELXTL*; software used to prepare material for publication: *XCIF* in *SHELXTL*.

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