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Bis[μ-2-(2-oxidobenzoylhydrazono)propanoato]bis{aqua[2-(2-hydroxybenzoylhydrazono)propanoato]yttrium(III)} bis{pentaaqua[2-(2-oxidobenzoylhydrazono)propanoato(3–)]yttrium(III)} hexahydrate

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The crystal structure of the title compound, $[Y_2(C_{10}H_8N_2O_4)_2(C_{10}H_9N_2O_4)_2(H_2O)_2][Y(C_{10}H_7N_2O_4)(H_2O)_5]_2\cdot6H_2O$, contains two independent molecular units, *viz*. a centrosymmetric dimeric $[Y(C_{20}H_8N_4O_8)_2(H_2O)]_2$ unit and a single $[Y(C_{10}H_7N_2O_4)(H_2O)_5]$ unit. Both Y^{III} ions have coordination number 8, with distorted dodecahedra as coordination polyhedra. Numerous intermolecular hydrogen bonds link the molecular units and three additional independent water molecules into a three-dimensional network.

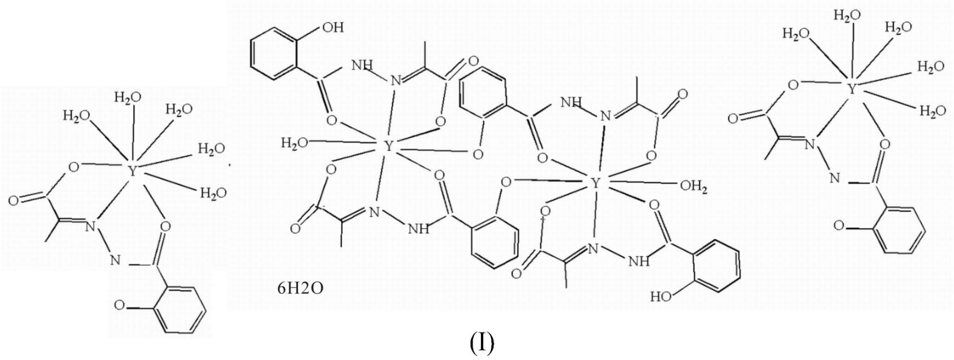
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
Some non-H atoms missing
R factor = 0.044
wR factor = 0.114
Data-to-parameter ratio = 11.3

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

Comment

Hydrazones have attracted considerable attention due to their coordination behaviour and pharmacological activity. Many physiologically active hydrazone–metal complexes find application in the treatment of several diseases, such as tuberculosis and cancer (Rodriguez-Argelles *et al.*, 2004; Buss *et al.*, 2003). *N*-(2-Propionic acid)salicyloyl hydrazone ($C_{10}H_{10}N_2O_4$) can act as a bridging ligand in a μ_2 coordination mode *via* its carboxyl O atoms (Wu *et al.*, 2006), or it can act as a tridentate chelating ligand (He *et al.*, 2005). It is interesting to note that, in the title compound, (I), this ligand acts in a different coordination mode; in a part of the structure the bridging is realised by the phenolic O atom.



(I)

In compound (I), two crystallographically independent molecular units are present (Fig. 1), a centrosymmetric dimeric $[Y(C_{20}H_{17}N_4O_8)(H_2O)]_2$ unit and a single $[Y(C_{10}H_7N_2O_4)(H_2O)_5]$ unit. The coordination polyhedra around both Y^{III} ions may be described as distorted dodecahedra. However, the coordination environments are different in the two units. In the single unit, Y is surrounded by one N and seven O atoms, [Y2NO$_7$], whereas in the dimeric unit, Y is coordinated by two N atoms of two different ligands and by six

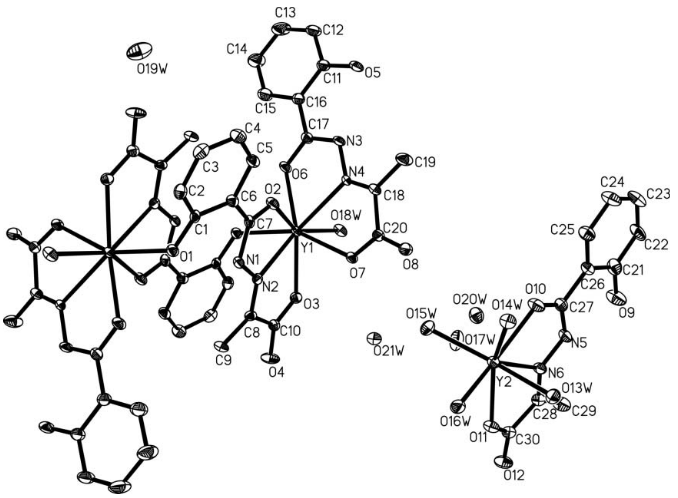


Figure 1

A view of the molecular units of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

O atoms, [Y1N$_2$O$_6$]. The mean Y—O bond length of 2.342 Å is considerably shorter than that of Y—N (2.479 Å).

The bond lengths of O2—C7, O10—C27 and O6—C17 are 1.248 (5), 1.276 (6) and 1.272 (5) Å, respectively. When compared with the mean bond lengths for C—O bonds ($\simeq$1.42 Å; Chen & Cai, 2003) and for C═O bonds ($\simeq$1.23 Å; Chen & Cai, 2003), these can be clearly considered as double bonds, with keto groups as ligands to the Y atoms.

There are extensive hydrogen bonds in the crystal structure of (I), leading to a stabilization of the three-dimensional network. Additionally, all solvent water molecules (O19*W*, O20*W* and O21*W*) are linked with the ligands *via* moderate hydrogen bonds (Table 2).

Experimental

Yttrium(III) nitrate hydrate was prepared by dissolving Y_2O_3 in concentrated HNO_3 and subsequent crystallization. The ligand H_3L, *N*-(2-propionic acid)salicyloyl hydrazone, was prepared according to He *et al.* (2002). All chemicals used were of analytical grade, except pyruvic acid (biochemical reagent). The ligand H_3L and $Y(NO_3)_3 \cdot nH_2O$ (molar ratio 2:1) were dissolved in a water–ethanol mixture (1:2 *v*/*v*). The resultant solution was refluxed for 2 h and then filtered. The filtrate was left to evaporate for about three weeks at room temperature. Yellow prismatic crystals were obtained. The results of the elemental analysis are in good agreement with the composition of (I).

Crystal data

$[Y_2(C_{10}H_8N_2O_4)_2(C_{10}H_9N_2O_4)_2$-$(H_2O)_2][Y(C_{10}H_7N_2O_4)$-$(H_2O)_5]_2 \cdot 6H_2O$
$M_r = 2001.00$
Triclinic, $P\overline{1}$
$a = 7.7484$ (10) Å
$b = 14.746$ (2) Å
$c = 17.980$ (3) Å
$\alpha = 102.128$ (2)°
$\beta = 97.981$ (2)°
$\gamma = 90.351$ (2)°
$V = 1987.7$ (5) Å^3
$Z = 2$
$D_x = 1.672$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.00$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.46 × 0.39 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.360$, $T_{max} = 0.716$ (expected range = 0.193–0.384)
9888 measured reflections
6874 independent reflections
4815 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.114$
$S = 1.01$
6874 reflections
608 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.4536P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.72$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

Table 1

Selected bond lengths (Å).

Y1—O1^{i}	2.279 (3)	Y2—O10	2.276 (3)
Y1—O6	2.303 (3)	Y2—O11	2.323 (3)
Y1—O2	2.333 (3)	Y2—O13*W*	2.325 (4)
Y1—O3	2.351 (3)	Y2—O16*W*	2.347 (4)
Y1—O7	2.365 (3)	Y2—O17*W*	2.355 (4)
Y1—O18*W*	2.404 (4)	Y2—O15*W*	2.361 (4)
Y1—N4	2.485 (3)	Y2—O14*W*	2.434 (4)
Y1—N2	2.504 (4)	Y2—N6	2.449 (4)

Symmetry code: (i) $-x, -y+2, -z+1$.

Table 2

Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O19*W*—H19*E*···O4^{i}	0.851 (10)	2.10 (8)	2.746 (6)	132 (9)
O15*W*—H15*A*···O8	0.851 (10)	1.93 (2)	2.745 (5)	161 (6)
O17*W*—H17*B*···O21*W*	0.851 (10)	1.863 (17)	2.703 (6)	169 (7)
O17*W*—H17*A*···O20*W*	0.847 (10)	2.024 (19)	2.849 (6)	164 (6)
O14*W*—H14*A*···O18*W*^{ii}	0.850 (10)	2.224 (19)	3.065 (6)	170 (8)
O13*W*—H13*B*···O19*W*^{iii}	0.846 (10)	1.838 (14)	2.678 (6)	172 (6)
O19*W*—H19*D*···O12^{iv}	0.851 (10)	2.02 (3)	2.843 (6)	161 (7)
O13*W*—H13*A*···O20*W*^{ii}	0.843 (10)	1.914 (14)	2.751 (6)	172 (6)
O16*W*—H16*B*···O11^{v}	0.849 (11)	1.892 (14)	2.737 (5)	173 (7)
O16*W*—H16*A*···O19*W*^{vi}	0.851 (10)	2.67 (6)	3.065 (7)	110 (5)
O16*W*—H16*A*···O4^{ii}	0.851 (10)	2.19 (2)	3.006 (6)	161 (6)
O18*W*—H18*A*···O5^{vii}	0.849 (10)	1.871 (14)	2.714 (5)	172 (5)
O18*W*—H18*B*···O8^{viii}	0.847 (10)	1.988 (15)	2.826 (5)	170 (6)
O21*W*—H21*B*···O12^{ix}	0.848 (10)	1.913 (12)	2.759 (5)	176 (5)
O21*W*—H21*A*···O7	0.845 (10)	1.99 (2)	2.781 (5)	155 (5)
O20*W*—H20*B*···O10^{viii}	0.848 (10)	2.65 (4)	3.353 (6)	141 (5)
O20*W*—H20*A*···O9^{x}	0.845 (10)	1.98 (3)	2.779 (6)	157 (6)
O15*W*—H15*B*···O3^{ii}	0.852 (10)	1.917 (13)	2.765 (5)	173 (6)
O14*W*—H14*B*···O21*W*^{ii}	0.849 (10)	1.871 (16)	2.711 (5)	170 (6)
N1—H1···O1	0.86	2.08	2.678 (5)	126
O5—H5···N3	0.82	1.97	2.573 (5)	130

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x+1, y, z$; (iii) $x+1, y, z+1$; (iv) $x, y, z-1$; (v) $-x+2, -y+2, -z+2$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x, -y+1, -z+1$; (viii) $x-1, y, z$; (ix) $-x+1, -y+2, -z+2$; (x) $-x+1, -y+1, -z+2$.

The water H atoms were located in a difference Fourier map and refined with a distance restraint of O—H = 0.85 (1) Å. H atoms attached to C and N atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H, C—H = 0.96 Å for methyl H and N—H =

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0.86 Å. They were treated as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N) or 1.5$U_{\rm eq}$($C_{\rm methyl}$).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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m470 Chen *et al.* • $[Y_2(C_{10}H_8N_2O_4)_2(C_{10}H_9N_2O_4)_2][Y(C_{10}H_7N_2O_4)]_2$ *Acta Cryst.* (2007). E**63**, m468–m470