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catena-Poly[[tetrakis(hexamethylphosphoramide-κO)bis(nitrato-κ^2O,O')ytterbium(III)] [silver(I)-di-μ-sulfido-tungstate(VI)(*Ag*—*W*)-di-μ-sulfido]]

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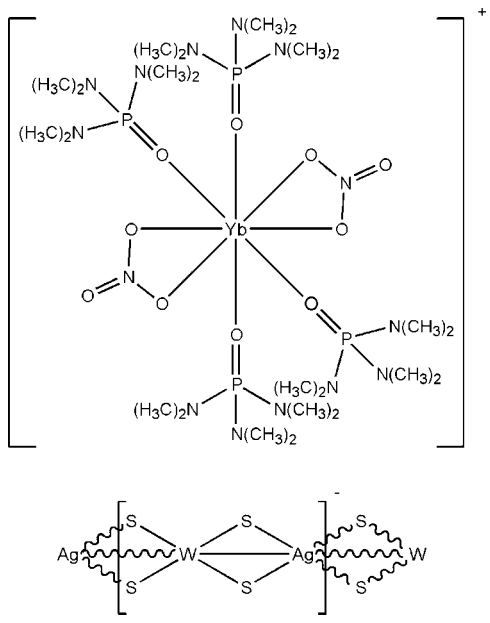
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(Ag–S) = 0.001 Å; R factor = 0.032; wR factor = 0.069; data-to-parameter ratio = 18.1.

The self-assembly of tetrathiotungstate(VI), silver sulfide and ytterbium(III) nitrate in hexamethylphosphoramide (hmp) resulted in a one-dimensional anionic W/S/Ag polymer, $\{[Yb(NO_3)_2(C_6H_{18}N_3OP)_4][WAgS_4]\}_n$. The central Yb coordination polyhedron in the cationic complex $[Yb(hmp)_4(NO_3)_2]^+$ is a distorted square antiprism. The $[YbO_8]$ assembly has an approximate fourfold inversion axis along the bisector of one of the chelating nitrate groups. The polymeric anion $\{[WS_4Ag]^-\}_n$ presents a distorted linear configuration, with W—Ag—W and Ag—W—Ag angles of 160.81 (7) and 153.41 (7)°, deviating significantly from the ideal 180°. The anionic chains in the title compound are similar to those in $\{N(C_6H_5CH_2)(C_2H_5)_3[MoS_4Ag]\}_n$: they both have a similar wave-like appearance but have different orientations. The former propagate along the c axis, while the latter have two orientations: one parallel to the a axis and the other parallel to the b axis.

Related literature

An example of a one-dimensional Mo/S/Ag anionic polymer with an almost ideal linear configuration is $\{(\gamma$-MePyH)[Mo$S_4Ag]\}_n$ (Lang *et al.*, 1993). A more relevant analog of the title compound is $\{N(C_6H_5CH_2)(C_2H_5)_3[MoS_4Ag]\}_n$ (Yu *et al.*, 1998), which has similar wave-like chains but with different chain orientations. For related literature, see: Huang *et al.* (1997); Niu *et al.* (2004).



Experimental

Crystal data

$[Yb(NO_3)_2(C_6H_{18}N_3OP)_4][WAgS_4]$
M_r = 1433.87
Monoclinic, $P2_1/c$
a = 15.7241 (9) Å
b = 29.5280 (18) Å
c = 11.3464 (7) Å
β = 90.798 (1)°
V = 5267.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.64 mm^{-1}
T = 153 (2) K
0.55 × 0.45 × 0.30 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.097, T_{max} = 0.243
47611 measured reflections
9611 independent reflections
9126 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.069
S = 1.18
9611 reflections
532 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −1.05 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Financial support from the National Natural Science Foundation of China (grant No. 50472048) and the Program for New Century Excellent Talents in Universities (grant No. NCET-05-0499) is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2049).

  doi:10.1107/S1600536807031480

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supplementary materials

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catena-Poly[[tetrakis(hexamethylphosphoramide-κO)bis(nitrato-$\kappa^2 O,O'$)ytterbium(III)] [silver(I)-di-μ-sulfido-tungstate(VI)(*Ag*-*W*)-di-μ-sulfido]]

Y. Cao, J.-F. Zhang, J. Qian and C. Zhang

Comment

One-dimensional Mo(W)/S/Ag anionic polymers are very impressive in light of configurational isomerism (Niu *et al.*, 2004, and references therein). Different solvent-coordinated rare earth cations proved effective to obtain various configurations of anionic chains (Niu *et al.*, 2004). The title compound $\{[Yb(hmp)_4(NO_3)_2][WS_4Ag]\}_n$ (hmp = hexamethylphosphoramide) with a wave-like anionic chain was prepared by following such route using Yb(III)-hmp complex as counterion.

The cationic complex in the title compound is univalent as a result of the inclusion of two nitrate ligands, hence inducing an anionic chain with a univalent repeat unit, unlike other solvent-coordinated rare earth cations in literature (Niu *et al.*, 2004), which are trivalent and induce trivalent repeat units. For example, $[Nd(dmso)_8]^{3+}$ induces a helical chain with a trivalent repeat unit $[W_3S_{12}Ag_3]^{3-}$ (Huang *et al.*, 1997).

The central Yb in the cationic complex $[Yb(hmp)_4(NO_3)_2]^+$ has distorted square antiprismatic coordination (Fig. 1). The eight O atoms from four hmp and two nitrate ligands may be sorted into two groups (O1, O3, O6, O7 and O2, O4, O8, O9), each group together with the central Yb nearly coplanar. The two planes formed by these two groups are perpendicular to each other. The $[YbO_8]$ assembly has an approximate 4-folded inversion axis along the bisector of the O6—Yb1—O7 angle (Fig. 2).

Fig. 3 shows a portion of the polymeric anion in the title compound, which has a distorted linear configuration with W—Ag—W and Ag—W—Ag angles of 160.81 (7) and 153.41 (7) ° heavily deviating from the ideal 180 °, which is observed in the reported compound $\{(\gamma\text{-MePyH})[MoS_4Ag]\}_n$ (179.3 (2)–180.0 (1) °) (Lang *et al.*, 1993). Similar angles of 156.47 (5) and 157.14 (5) ° for Mo—Ag—Mo and Ag—Mo—Ag are found in another distorted linear chain in $\{N(C_6H_5CH_2)(C_2H_5)_3[MoS_4Ag]\}_n$ (Yu *et al.*, 1998). The whole anionic chains in both the title compound and the compound above have similar wave-like appearance but with different orientations. The former propagates along the *c* axis, while the latter has two orientations: one parallel to *a* axis and the other parallel to *b* axis.

Experimental

0.5 mmol A g_2S was added to a solution of $[NH_4]_2WS_4$ (1 mmol in 20 mL h mp) with thorough stir for 10 h. The solution underwent an additional stir for one minute after 0.5 mmol $Yb(NO_3)_36H_2O$ was added. After filtration the orange-red filtrate was carefully laid on the surface with 20 ml *i*-PrOH. Red block crystals were obtained after ten days. Yield: 0.836 g in pure form, 58.3% (based on W). Analysis calculated for $C_{24}H_{72}AgN_{14}O_{10}P_4S_4WYb$: C 20.08, H 5.42, N 13.67%; found: C 20.44, H 5.57, N 13.38%. IR: ν, cm^{-1}, 480*m*, 447 s, 436s h (W-μ_2-S).

Refinement

A few C atoms and O5 have notably larger U_{eq} than others or have large ADP max/min ratio (Alert level C). Splitting these atoms to resolve disorder will cause the refinement unstable or ADP non positive definite, so no further treatments were applied to these atoms. H atoms were positioned geometrically and refined with riding model, with $U_{iso} = 1.5U_{eq}$ and C—H bond length 0.98 Å for methyl H atoms.

Figures

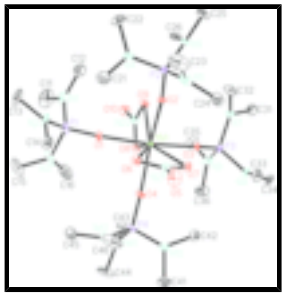

Fig. 1. The molecular structure of the cation in the title compound, with atom labels and 30% probability displacement ellipsoids. All H atoms have been omitted.

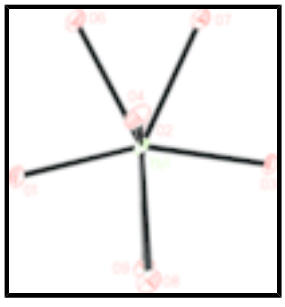

Fig. 2. The coordination geometry of the [YbO_8] assembly.

Fig. 3. The molecular structure of a portion of the anionic chain in the title compound, with atom labels and 30% probability displacement ellipsoids.

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Crystal data

$[Yb(NO_3)_2(C_6H_{18}N_3OP)_4][WAgS_4]$	$F_{000} = 2836$
$M_r = 1433.87$	$D_x = 1.808$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2ybc	Cell parameters from 17963 reflections
$a = 15.7241$ (9) Å	θ = 3.0–25.4°
$b = 29.5280$ (18) Å	μ = 4.64 mm^{-1}
$c = 11.3464$ (7) Å	$T = 153$ (2) K
β = 90.7980 (10)°	Block, red
$V = 5267.6$ (5) Å^3	0.55 × 0.45 × 0.30 mm
$Z = 4$	

Data collection

Rigaku Mercury CCD (2 x 2 bin mode) diffractometer	9611 independent reflections
Radiation source: fine-focus sealed tube	9126 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
$T = 153(2)$ K	$\theta_{max} = 25.4^{o}$
dtprofit.ref scans	$\theta_{min} = 3.0^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -17 \rightarrow 18$
$T_{min} = 0.097$, $T_{max} = 0.243$	$k = -35 \rightarrow 35$
47611 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.017P)^2 + 19.3445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.18$	$(\Delta/\sigma)_{max} = 0.002$
9611 reflections	$\Delta\rho_{max} = 0.93$ e Å^{-3}
532 parameters	$\Delta\rho_{min} = -1.04$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Yb1	0.238238 (12)	0.082437 (7)	0.826783 (18)	0.01266 (6)
P1	0.29365 (10)	0.14628 (5)	1.09340 (12)	0.0261 (3)
P2	0.02328 (8)	0.13163 (5)	0.82032 (11)	0.0188 (3)
P3	0.20073 (8)	−0.03022 (4)	0.70195 (11)	0.0188 (3)
P4	0.45674 (8)	0.09666 (4)	0.73072 (12)	0.0184 (3)

O2	0.10510 (19)	0.10586 (11)	0.8224 (3)	0.0185 (7)
O4	0.3741 (2)	0.08048 (11)	0.7800 (3)	0.0213 (8)
O3	0.2073 (2)	0.01886 (11)	0.7298 (3)	0.0187 (7)
O1	0.2719 (2)	0.12614 (11)	0.9769 (3)	0.0205 (8)
O5	0.2267 (3)	0.17135 (14)	0.5539 (4)	0.0495 (12)
O6	0.2519 (2)	0.15767 (11)	0.7393 (3)	0.0225 (8)
O7	0.2241 (2)	0.10250 (11)	0.6210 (3)	0.0225 (8)
O8	0.3020 (2)	0.02711 (12)	0.9616 (3)	0.0216 (8)
O9	0.1695 (2)	0.04121 (12)	0.9860 (3)	0.0207 (8)
O10	0.2385 (3)	0.00200 (14)	1.1183 (3)	0.0351 (10)
N8	0.2224 (3)	−0.03703 (15)	0.5613 (4)	0.0247 (10)
N7	0.1072 (3)	−0.04816 (16)	0.7417 (4)	0.0324 (12)
N9	0.2668 (3)	−0.06466 (15)	0.7692 (4)	0.0289 (11)
N10	0.4539 (3)	0.08728 (17)	0.5880 (4)	0.0302 (11)
N11	0.5331 (3)	0.07057 (16)	0.8027 (4)	0.0296 (11)
N12	0.4823 (3)	0.14966 (15)	0.7396 (4)	0.0308 (11)
N3	0.3956 (3)	0.13927 (18)	1.1205 (5)	0.0464 (15)
N1	0.2403 (4)	0.12298 (18)	1.1978 (4)	0.0438 (14)
N5	0.0076 (3)	0.15537 (19)	0.6931 (4)	0.0369 (13)
N4	0.0235 (3)	0.17178 (16)	0.9188 (4)	0.0325 (11)
N6	−0.0541 (3)	0.09614 (15)	0.8465 (4)	0.0226 (10)
N21	0.2344 (3)	0.14476 (15)	0.6356 (4)	0.0246 (10)
N22	0.2367 (3)	0.02247 (14)	1.0250 (4)	0.0211 (9)
N2	0.2722 (3)	0.20015 (15)	1.0922 (4)	0.0328 (12)
C41	0.5280 (4)	0.0972 (3)	0.5153 (6)	0.053 (2)
H41A	0.5150	0.0895	0.4329	0.079*
H41B	0.5766	0.0792	0.5431	0.079*
H41C	0.5419	0.1294	0.5212	0.079*
C11	0.2776 (7)	0.1064 (3)	1.3076 (6)	0.084 (3)
H11A	0.2328	0.0938	1.3570	0.126*
H11B	0.3056	0.1315	1.3493	0.126*
H11C	0.3194	0.0828	1.2905	0.126*
C42	0.4062 (4)	0.0479 (2)	0.5434 (5)	0.0376 (15)
H42A	0.3573	0.0423	0.5939	0.056*
H42B	0.4433	0.0212	0.5438	0.056*
H42C	0.3863	0.0539	0.4627	0.056*
C43	0.5204 (4)	0.0278 (2)	0.8610 (6)	0.0465 (18)
H43A	0.5737	0.0181	0.8990	0.070*
H43B	0.5024	0.0050	0.8029	0.070*
H43C	0.4764	0.0311	0.9207	0.070*
C45	0.5143 (5)	0.1695 (3)	0.8496 (7)	0.058 (2)
H45A	0.5260	0.2017	0.8376	0.087*
H45B	0.5668	0.1540	0.8740	0.087*
H45C	0.4715	0.1660	0.9110	0.087*
C46	0.4502 (4)	0.1842 (2)	0.6566 (8)	0.058 (2)
H46A	0.4295	0.1695	0.5844	0.088*
H46B	0.4963	0.2052	0.6374	0.088*
H46C	0.4036	0.2010	0.6929	0.088*
C23	−0.0359 (5)	0.1997 (3)	0.6780 (7)	0.062 (2)

H23A	−0.0386	0.2075	0.5940	0.093*
H23B	−0.0041	0.2231	0.7210	0.093*
H23C	−0.0937	0.1977	0.7088	0.093*
C24	0.0203 (4)	0.1299 (3)	0.5860 (6)	0.065 (3)
H24A	0.0489	0.1013	0.6049	0.098*
H24B	0.0555	0.1475	0.5322	0.098*
H24C	−0.0349	0.1236	0.5483	0.098*
C25	−0.1423 (3)	0.1056 (2)	0.8095 (5)	0.0366 (15)
H25A	−0.1790	0.0805	0.8335	0.055*
H25B	−0.1453	0.1090	0.7237	0.055*
H25C	−0.1616	0.1337	0.8469	0.055*
C21	0.0897 (4)	0.2067 (2)	0.9178 (7)	0.0493 (18)
H21A	0.0803	0.2281	0.9824	0.074*
H21B	0.0874	0.2229	0.8425	0.074*
H21C	0.1456	0.1924	0.9279	0.074*
C22	−0.0466 (4)	0.1823 (2)	0.9967 (6)	0.0440 (17)
H22A	−0.0885	0.1577	0.9934	0.066*
H22B	−0.0736	0.2107	0.9715	0.066*
H22C	−0.0249	0.1855	1.0776	0.066*
C33	0.1965 (4)	−0.0027 (2)	0.4767 (5)	0.0369 (14)
H33A	0.2141	−0.0118	0.3977	0.055*
H33B	0.2234	0.0262	0.4976	0.055*
H33C	0.1345	0.0007	0.4778	0.055*
C34	0.2277 (4)	−0.0827 (2)	0.5100 (5)	0.0356 (14)
H34A	0.2453	−0.1043	0.5712	0.053*
H34B	0.2694	−0.0828	0.4466	0.053*
H34C	0.1718	−0.0915	0.4781	0.053*
C31	0.0825 (5)	−0.0956 (2)	0.7234 (6)	0.0499 (19)
H31A	0.0246	−0.1003	0.7520	0.075*
H31B	0.1220	−0.1154	0.7668	0.075*
H31C	0.0844	−0.1028	0.6392	0.075*
C32	0.0357 (4)	−0.0167 (2)	0.7454 (6)	0.0444 (17)
H32A	0.0571	0.0142	0.7579	0.067*
H32B	−0.0018	−0.0250	0.8101	0.067*
H32C	0.0039	−0.0180	0.6705	0.067*
C35	0.2548 (5)	−0.0807 (2)	0.8884 (6)	0.0486 (18)
H35A	0.3019	−0.1008	0.9109	0.073*
H35B	0.2010	−0.0974	0.8925	0.073*
H35C	0.2533	−0.0549	0.9424	0.073*
C12	0.1489 (5)	0.1192 (3)	1.1865 (6)	0.058 (2)
H12A	0.1303	0.1313	1.1100	0.088*
H12B	0.1220	0.1364	1.2498	0.088*
H12C	0.1323	0.0873	1.1922	0.088*
C15	0.4495 (5)	0.1718 (3)	1.1833 (8)	0.073 (3)
H15A	0.5078	0.1601	1.1885	0.109*
H15B	0.4277	0.1765	1.2628	0.109*
H15C	0.4493	0.2007	1.1407	0.109*
C16	0.4355 (5)	0.0951 (3)	1.1066 (7)	0.058 (2)
H16A	0.3965	0.0747	1.0642	0.087*

H16B	0.4490	0.0824	1.1844	0.087*
H16C	0.4880	0.0984	1.0618	0.087*
C44	0.6223 (4)	0.0802 (3)	0.7801 (7)	0.053 (2)
H44A	0.6271	0.1097	0.7410	0.080*
H44B	0.6456	0.0566	0.7292	0.080*
H44C	0.6542	0.0808	0.8549	0.080*
C36	0.3559 (4)	−0.0672 (3)	0.7363 (7)	0.0518 (19)
H36A	0.3623	−0.0562	0.6555	0.078*
H36B	0.3752	−0.0987	0.7412	0.078*
H36C	0.3902	−0.0485	0.7902	0.078*
C26	−0.0455 (3)	0.0637 (2)	0.9430 (5)	0.0301 (13)
H26A	0.0149	0.0593	0.9622	0.045*
H26B	−0.0707	0.0347	0.9192	0.045*
H26C	−0.0748	0.0753	1.0124	0.045*
C13	0.2469 (6)	0.2259 (2)	1.1959 (6)	0.062 (2)
H13A	0.2372	0.2576	1.1738	0.094*
H13B	0.2921	0.2243	1.2561	0.094*
H13C	0.1944	0.2131	1.2274	0.094*
C14	0.3010 (4)	0.22756 (19)	0.9925 (5)	0.0350 (14)
H14A	0.3163	0.2076	0.9271	0.052*
H14B	0.3508	0.2454	1.0169	0.052*
H14C	0.2552	0.2480	0.9669	0.052*
W1	0.716929 (12)	0.227369 (6)	0.473839 (16)	0.01396 (6)
Ag1	0.71835 (3)	0.233860 (14)	0.21310 (3)	0.02776 (10)
S1	0.60322 (8)	0.21167 (5)	0.36755 (11)	0.0262 (3)
S2	0.83218 (8)	0.21133 (5)	0.37351 (11)	0.0247 (3)
S3	0.71644 (9)	0.30071 (4)	0.51273 (11)	0.0235 (3)
S4	0.71521 (8)	0.18478 (4)	0.63354 (11)	0.0216 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb1	0.01101 (11)	0.00816 (10)	0.01884 (11)	−0.00037 (7)	0.00089 (8)	−0.00117 (8)
P1	0.0399 (9)	0.0151 (7)	0.0231 (7)	−0.0076 (6)	−0.0123 (6)	−0.0008 (6)
P2	0.0123 (6)	0.0237 (7)	0.0206 (7)	0.0034 (5)	0.0008 (5)	0.0049 (5)
P3	0.0238 (7)	0.0115 (7)	0.0211 (7)	−0.0039 (5)	0.0058 (5)	−0.0049 (5)
P4	0.0122 (6)	0.0158 (7)	0.0271 (7)	−0.0001 (5)	0.0030 (5)	0.0056 (5)
O2	0.0125 (17)	0.0172 (19)	0.0258 (19)	0.0036 (13)	0.0022 (14)	−0.0010 (14)
O4	0.0151 (18)	0.0153 (18)	0.034 (2)	−0.0028 (14)	0.0050 (15)	0.0035 (15)
O3	0.0245 (19)	0.0094 (17)	0.0223 (18)	−0.0024 (14)	0.0001 (14)	−0.0050 (14)
O1	0.0227 (19)	0.0143 (18)	0.0243 (19)	−0.0020 (14)	−0.0056 (14)	−0.0043 (14)
O5	0.084 (4)	0.026 (2)	0.038 (3)	−0.010 (2)	−0.012 (2)	0.018 (2)
O6	0.026 (2)	0.0129 (19)	0.028 (2)	−0.0024 (14)	−0.0002 (15)	0.0010 (15)
O7	0.030 (2)	0.0136 (19)	0.0237 (19)	−0.0003 (15)	0.0021 (15)	0.0001 (15)
O8	0.0158 (18)	0.0185 (19)	0.030 (2)	−0.0004 (14)	0.0014 (15)	0.0017 (15)
O9	0.0168 (18)	0.0175 (19)	0.028 (2)	−0.0015 (14)	0.0008 (14)	0.0031 (15)
O10	0.039 (2)	0.036 (2)	0.030 (2)	−0.0021 (19)	−0.0018 (18)	0.0169 (19)
N8	0.036 (3)	0.018 (2)	0.021 (2)	−0.0039 (19)	0.0079 (19)	−0.0059 (18)

N7	0.028 (3)	0.026 (3)	0.043 (3)	−0.010 (2)	0.012 (2)	−0.011 (2)
N9	0.043 (3)	0.014 (2)	0.029 (3)	0.006 (2)	0.011 (2)	0.0042 (19)
N10	0.023 (2)	0.041 (3)	0.027 (3)	−0.006 (2)	0.0049 (19)	0.004 (2)
N11	0.014 (2)	0.034 (3)	0.041 (3)	−0.0002 (19)	0.0045 (19)	0.021 (2)
N12	0.025 (3)	0.017 (2)	0.051 (3)	−0.0044 (19)	0.009 (2)	0.002 (2)
N3	0.046 (3)	0.031 (3)	0.062 (4)	−0.012 (2)	−0.034 (3)	0.001 (3)
N1	0.072 (4)	0.033 (3)	0.027 (3)	−0.018 (3)	−0.002 (3)	0.007 (2)
N5	0.022 (3)	0.057 (4)	0.032 (3)	0.000 (2)	−0.007 (2)	0.021 (3)
N4	0.021 (2)	0.029 (3)	0.048 (3)	0.005 (2)	0.009 (2)	−0.009 (2)
N6	0.012 (2)	0.032 (3)	0.024 (2)	−0.0010 (18)	0.0002 (17)	0.0026 (19)
N21	0.029 (3)	0.016 (2)	0.029 (3)	−0.0017 (18)	−0.0002 (19)	0.006 (2)
N22	0.022 (2)	0.017 (2)	0.024 (2)	−0.0031 (18)	−0.0016 (19)	0.0028 (18)
N2	0.066 (4)	0.013 (2)	0.019 (2)	−0.005 (2)	0.006 (2)	−0.0069 (19)
C41	0.043 (4)	0.079 (6)	0.037 (4)	−0.016 (4)	0.013 (3)	0.011 (4)
C11	0.136 (9)	0.088 (7)	0.028 (4)	−0.009 (6)	−0.004 (5)	0.018 (4)
C42	0.034 (3)	0.044 (4)	0.035 (3)	−0.001 (3)	0.001 (3)	−0.005 (3)
C43	0.025 (3)	0.047 (4)	0.068 (5)	0.006 (3)	0.003 (3)	0.037 (4)
C45	0.064 (5)	0.044 (4)	0.066 (5)	−0.031 (4)	0.021 (4)	−0.018 (4)
C46	0.034 (4)	0.027 (4)	0.114 (7)	0.002 (3)	0.007 (4)	0.040 (4)
C23	0.045 (4)	0.062 (5)	0.079 (6)	0.013 (4)	−0.012 (4)	0.047 (4)
C24	0.037 (4)	0.134 (8)	0.025 (4)	−0.015 (4)	−0.007 (3)	0.005 (4)
C25	0.018 (3)	0.050 (4)	0.042 (4)	−0.001 (3)	−0.004 (2)	0.011 (3)
C21	0.041 (4)	0.034 (4)	0.072 (5)	−0.002 (3)	0.012 (3)	−0.009 (3)
C22	0.044 (4)	0.036 (4)	0.053 (4)	0.012 (3)	0.020 (3)	−0.004 (3)
C33	0.050 (4)	0.033 (4)	0.027 (3)	−0.003 (3)	−0.007 (3)	0.000 (3)
C34	0.049 (4)	0.028 (3)	0.031 (3)	−0.006 (3)	0.014 (3)	−0.016 (3)
C31	0.059 (5)	0.037 (4)	0.055 (4)	−0.029 (3)	0.022 (3)	−0.014 (3)
C32	0.024 (3)	0.044 (4)	0.065 (5)	−0.002 (3)	0.000 (3)	0.007 (3)
C35	0.065 (5)	0.038 (4)	0.043 (4)	0.019 (3)	0.007 (3)	0.013 (3)
C12	0.069 (5)	0.056 (5)	0.051 (4)	−0.030 (4)	0.026 (4)	−0.010 (4)
C15	0.073 (6)	0.063 (6)	0.081 (6)	−0.033 (4)	−0.036 (5)	0.004 (5)
C16	0.042 (4)	0.050 (5)	0.082 (6)	0.002 (3)	−0.028 (4)	0.011 (4)
C44	0.016 (3)	0.074 (5)	0.070 (5)	−0.001 (3)	0.002 (3)	0.049 (4)
C36	0.037 (4)	0.058 (5)	0.061 (5)	0.018 (3)	0.007 (3)	0.012 (4)
C26	0.019 (3)	0.037 (3)	0.034 (3)	−0.003 (2)	0.008 (2)	0.007 (3)
C13	0.121 (7)	0.031 (4)	0.036 (4)	−0.024 (4)	0.025 (4)	−0.019 (3)
C14	0.056 (4)	0.019 (3)	0.030 (3)	−0.007 (3)	0.007 (3)	−0.002 (2)
W1	0.01795 (11)	0.01220 (10)	0.01170 (10)	−0.00201 (7)	−0.00149 (7)	0.00054 (7)
Ag1	0.0456 (3)	0.0249 (2)	0.0128 (2)	−0.00002 (18)	−0.00088 (17)	0.00176 (16)
S1	0.0221 (7)	0.0358 (8)	0.0206 (7)	−0.0109 (6)	−0.0054 (5)	0.0027 (6)
S2	0.0228 (7)	0.0307 (8)	0.0206 (7)	0.0043 (5)	0.0011 (5)	0.0018 (6)
S3	0.0388 (8)	0.0127 (6)	0.0190 (6)	−0.0018 (5)	−0.0003 (5)	0.0006 (5)
S4	0.0333 (7)	0.0148 (6)	0.0166 (6)	0.0012 (5)	0.0001 (5)	0.0040 (5)

Geometric parameters (Å, °)

W1—S1	2.1923 (13)	P4—O4	1.500 (3)
W1—S2	2.2050 (13)	P4—N12	1.618 (5)
W1—S4	2.2061 (12)	P4—N11	1.636 (4)

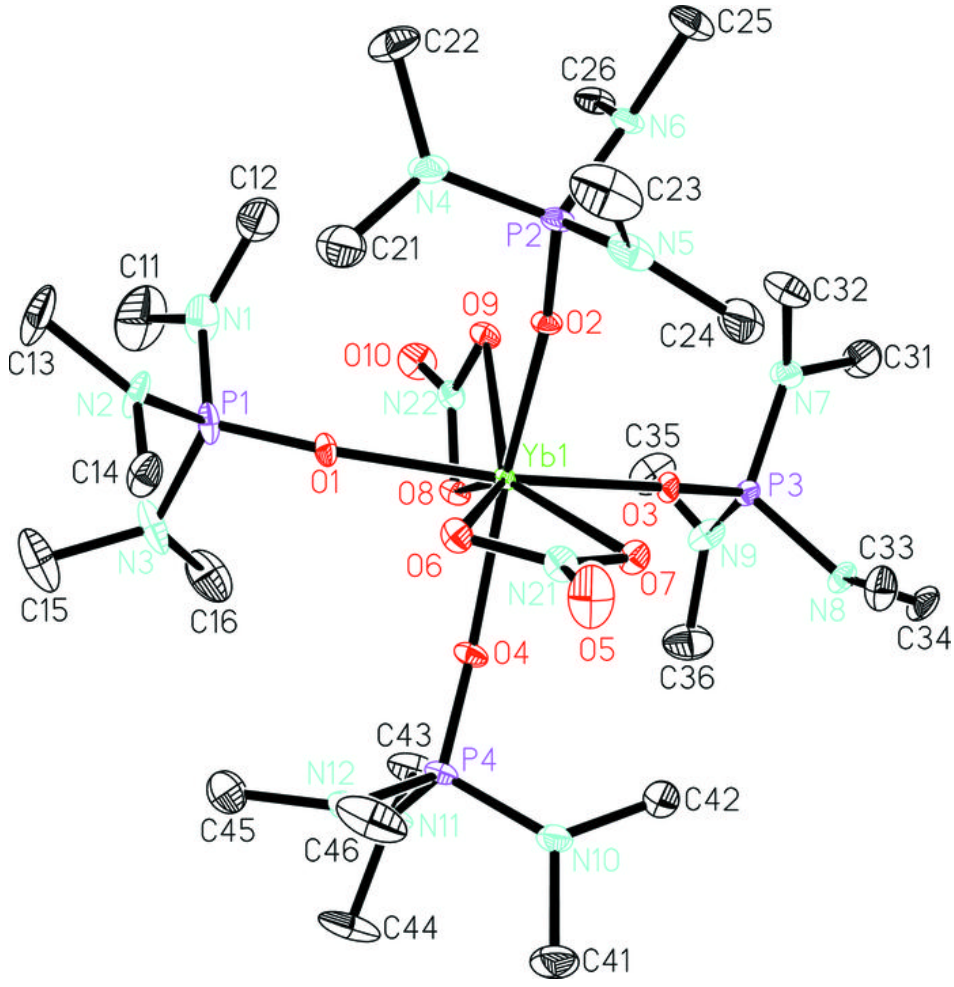
W1—S3	2.2102 (13)	P4—N10	1.643 (5)
W1—Ag1^{i}	2.9461 (5)	O5—N21	1.219 (6)
W1—Ag1	2.9650 (5)	O6—N21	1.263 (5)
Ag1—S3^{ii}	2.4920 (13)	O7—N21	1.269 (5)
Ag1—S4^{ii}	2.5667 (13)	O8—N22	1.270 (5)
Ag1—S1	2.6203 (14)	O9—N22	1.267 (5)
Ag1—S2	2.6207 (14)	O10—N22	1.220 (5)
Ag1—W1^{ii}	2.9461 (5)	N1—C12	1.445 (9)
S3—Ag1^{i}	2.4920 (13)	N1—C11	1.455 (9)
S4—Ag1^{i}	2.5667 (13)	N2—C13	1.461 (8)
Yb1—O1	2.196 (3)	N2—C14	1.468 (7)
Yb1—O2	2.205 (3)	N3—C16	1.458 (9)
Yb1—O4	2.210 (3)	N3—C15	1.461 (8)
Yb1—O3	2.227 (3)	N4—C22	1.455 (7)
Yb1—O7	2.416 (3)	N4—C21	1.464 (8)
Yb1—O9	2.443 (3)	N5—C24	1.446 (9)
Yb1—O8	2.444 (3)	N5—C23	1.486 (8)
Yb1—O6	2.444 (3)	N6—C26	1.461 (7)
Yb1—N21	2.845 (4)	N6—C25	1.471 (6)
Yb1—N22	2.862 (4)	N7—C32	1.459 (8)
P1—O1	1.485 (4)	N7—C31	1.468 (7)
P1—N1	1.615 (5)	N8—C33	1.451 (7)
P1—N2	1.626 (5)	N8—C34	1.472 (7)
P1—N3	1.640 (5)	N9—C35	1.448 (8)
P2—O2	1.495 (3)	N9—C36	1.457 (8)
P2—N5	1.620 (5)	N10—C41	1.466 (7)
P2—N4	1.629 (5)	N10—C42	1.470 (8)
P2—N6	1.636 (4)	N11—C43	1.441 (7)
P3—O3	1.487 (3)	N11—C44	1.457 (7)
P3—N7	1.633 (5)	N12—C45	1.461 (8)
P3—N9	1.635 (5)	N12—C46	1.473 (8)
P3—N8	1.649 (4)		
S1—W1—S2	109.91 (5)	O1—P1—N2	109.8 (2)
S1—W1—S4	108.19 (5)	N1—P1—N2	108.2 (3)
S2—W1—S4	108.73 (5)	O1—P1—N3	109.1 (3)
S1—W1—S3	108.18 (5)	N1—P1—N3	109.0 (3)
S2—W1—S3	108.58 (5)	N2—P1—N3	109.1 (3)
S4—W1—S3	113.23 (5)	O2—P2—N5	110.8 (2)
S1—W1—Ag1^{i}	125.79 (4)	O2—P2—N4	111.5 (2)
S2—W1—Ag1^{i}	124.29 (4)	N5—P2—N4	107.1 (3)
S4—W1—Ag1^{i}	57.63 (3)	O2—P2—N6	108.3 (2)
S3—W1—Ag1^{i}	55.62 (3)	N5—P2—N6	109.5 (2)
S1—W1—Ag1	58.82 (4)	N4—P2—N6	109.6 (2)
S2—W1—Ag1	58.74 (3)	O3—P3—N7	108.5 (2)
S4—W1—Ag1	148.95 (4)	O3—P3—N9	117.7 (2)
S3—W1—Ag1	97.81 (3)	N7—P3—N9	103.8 (3)

Ag1^{i}—W1—Ag1	153.412 (8)	O3—P3—N8	108.1 (2)
S3^{ii}—Ag1—S4^{ii}	93.59 (4)	N7—P3—N8	115.3 (2)
S3^{ii}—Ag1—S1	120.54 (5)	N9—P3—N8	103.7 (2)
S4^{ii}—Ag1—S1	117.33 (5)	O4—P4—N12	120.0 (2)
S3^{ii}—Ag1—S2	121.94 (5)	O4—P4—N11	107.3 (2)
S4^{ii}—Ag1—S2	119.44 (5)	N12—P4—N11	104.1 (3)
S1—Ag1—S2	86.77 (4)	O4—P4—N10	107.6 (2)
S3^{ii}—Ag1—W1^{ii}	47.05 (3)	N12—P4—N10	103.2 (3)
S4^{ii}—Ag1—W1^{ii}	46.55 (3)	N11—P4—N10	115.0 (3)
S1—Ag1—W1^{ii}	135.81 (3)	P1—O1—Yb1	167.4 (2)
S2—Ag1—W1^{ii}	137.30 (3)	P2—O2—Yb1	167.7 (2)
S3^{ii}—Ag1—W1	152.09 (3)	P3—O3—Yb1	160.2 (2)
S4^{ii}—Ag1—W1	114.27 (3)	P4—O4—Yb1	157.9 (2)
S1—Ag1—W1	45.71 (3)	N21—O6—Yb1	94.9 (3)
S2—Ag1—W1	45.99 (3)	N21—O7—Yb1	96.0 (3)
W1^{ii}—Ag1—W1	160.819 (16)	N22—O8—Yb1	95.6 (3)
W1—S1—Ag1	75.48 (4)	N22—O9—Yb1	95.7 (3)
W1—S2—Ag1	75.27 (4)	C12—N1—C11	116.0 (6)
W1—S3—Ag1^{i}	77.33 (4)	C12—N1—P1	119.6 (5)
W1—S4—Ag1^{i}	75.81 (4)	C11—N1—P1	124.3 (6)
O1—Yb1—O2	92.97 (12)	C13—N2—C14	115.1 (5)
O1—Yb1—O4	88.73 (13)	C13—N2—P1	124.2 (4)
O2—Yb1—O4	157.51 (13)	C14—N2—P1	118.6 (4)
O1—Yb1—O3	158.07 (13)	C16—N3—C15	113.1 (6)
O2—Yb1—O3	93.00 (12)	C16—N3—P1	120.9 (4)
O4—Yb1—O3	93.72 (12)	C15—N3—P1	124.6 (6)
O1—Yb1—O7	128.57 (12)	C22—N4—C21	113.5 (5)
O2—Yb1—O7	80.04 (12)	C22—N4—P2	125.3 (4)
O4—Yb1—O7	81.39 (12)	C21—N4—P2	120.1 (4)
O3—Yb1—O7	73.29 (12)	C24—N5—C23	115.5 (6)
O1—Yb1—O9	79.85 (12)	C24—N5—P2	120.2 (5)
O2—Yb1—O9	75.11 (12)	C23—N5—P2	123.3 (5)
O4—Yb1—O9	127.15 (12)	C26—N6—C25	114.6 (4)
O3—Yb1—O9	81.33 (12)	C26—N6—P2	119.7 (3)
O7—Yb1—O9	143.24 (11)	C25—N6—P2	121.8 (4)
O1—Yb1—O8	79.33 (12)	C32—N7—C31	114.2 (5)
O2—Yb1—O8	127.23 (12)	C32—N7—P3	119.8 (4)
O4—Yb1—O8	75.11 (12)	C31—N7—P3	120.5 (4)
O3—Yb1—O8	80.26 (12)	C33—N8—C34	113.3 (4)
O7—Yb1—O8	143.14 (12)	C33—N8—P3	119.7 (4)
O9—Yb1—O8	52.13 (11)	C34—N8—P3	120.5 (4)
O1—Yb1—O6	76.08 (12)	C35—N9—C36	111.1 (5)
O2—Yb1—O6	78.13 (12)	C35—N9—P3	123.3 (4)
O4—Yb1—O6	80.54 (12)	C36—N9—P3	121.3 (4)
O3—Yb1—O6	125.83 (12)	C41—N10—C42	111.7 (5)
O7—Yb1—O6	52.54 (12)	C41—N10—P4	120.7 (4)

O9—Yb1—O6	142.71 (12)	C42—N10—P4	118.7 (4)
O8—Yb1—O6	145.54 (11)	C43—N11—C44	113.1 (5)
O1—Yb1—N21	102.33 (13)	C43—N11—P4	122.4 (4)
O2—Yb1—N21	76.69 (12)	C44—N11—P4	121.5 (4)
O4—Yb1—N21	81.04 (13)	C45—N12—C46	112.3 (6)
O3—Yb1—N21	99.58 (12)	C45—N12—P4	121.5 (4)
O7—Yb1—N21	26.34 (12)	C46—N12—P4	123.2 (5)
O9—Yb1—N21	151.79 (12)	O5—N21—O6	122.1 (5)
O8—Yb1—N21	156.07 (12)	O5—N21—O7	121.5 (5)
O6—Yb1—N21	26.25 (12)	O6—N21—O7	116.4 (4)
O1—Yb1—N22	76.05 (12)	O5—N21—Yb1	175.6 (4)
O2—Yb1—N22	101.13 (12)	O6—N21—Yb1	58.9 (2)
O4—Yb1—N22	101.04 (12)	O7—N21—Yb1	57.7 (2)
O3—Yb1—N22	82.10 (12)	O10—N22—O9	121.9 (4)
O7—Yb1—N22	155.38 (12)	O10—N22—O8	122.4 (4)
O9—Yb1—N22	26.12 (11)	O9—N22—O8	115.7 (4)
O8—Yb1—N22	26.20 (11)	O10—N22—Yb1	171.3 (4)
O6—Yb1—N22	152.04 (12)	O9—N22—Yb1	58.1 (2)
N21—Yb1—N22	177.28 (13)	O8—N22—Yb1	58.2 (2)
O1—P1—N1	111.5 (2)		

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2.

Fig. 1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C31
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N9
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07
N8
C34
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04
C36
C43
P4
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C45
N11
C46
N10
C44
C41

Fig. 2

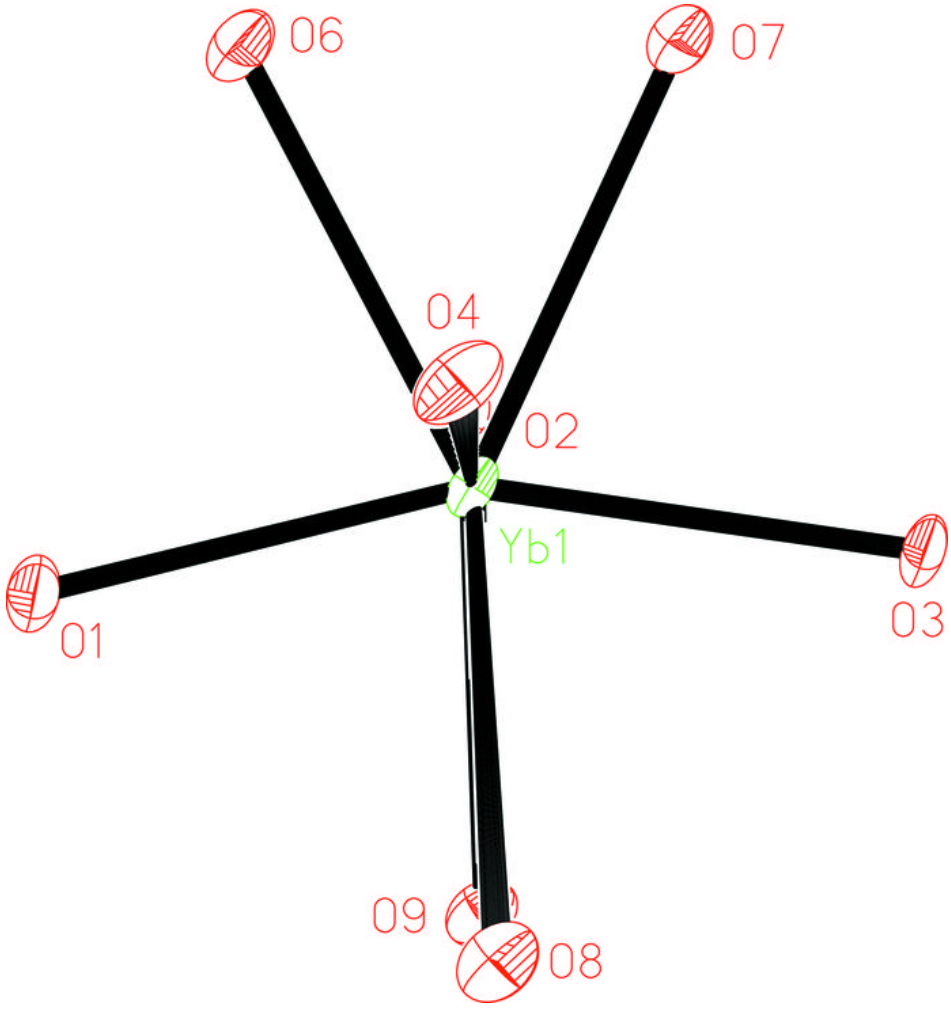

Fig. 3