

catena-Poly[[tetrakis(hexamethylphosphoramido-κO)bis(nitrato-κ²O,O')-erbium(III)] [silver(I)-di-μ-sulfido-tungstate(VI)-di-μ-sulfido]]

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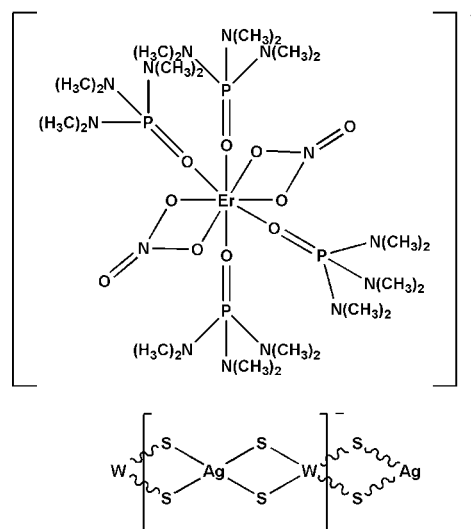
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{N}-\text{C}) = 0.012$ Å; R factor = 0.047; wR factor = 0.092; data-to-parameter ratio = 18.0.

In the title compound, $\{[\text{Er}(\text{NO}_3)_2(\text{C}_6\text{H}_{18}\text{N}_3\text{OP})_4][\text{AgWS}_4]\}_n$, the polymeric anionic chain $\{[\text{AgWS}_4]\}_n^-$ extends along $[001]$. The Er^{III} atom in the cation is coordinated by eight O atoms from two bidentate nitrate anions and four hexamethylphosphoramido ligands in a distorted square-antiprismatic geometry. Together with the two nitrate ligands, the cation is monovalent, which leads to the anionic chain having a $[\text{WS}_4\text{Ag}]$ repeat unit. The polymeric anionic chain has a distorted linear configuration, with $\text{W}-\text{Ag}-\text{W}$ and $\text{Ag}-\text{W}-\text{Ag}$ angles of $161.37(2)$ and $153.548(12)^\circ$, respectively. The title complex is isotypic with the Y, Yb, Eu, Nd, La, Dy, Sm, Lu and Tb analogues.

Related literature

For one-dimensional Mo(W)/S/Ag anionic polymers, see: Niu *et al.* (2004); Zhang *et al.* (2010). For their unique properties, see: Zhang, Song *et al.* (2007). For isotypic compounds, see: Zhang, Cao *et al.* (2007); Cao *et al.* (2007); Zhang, Qian *et al.* (2007); Tang, Zhang & Zhang (2008); Tang, Zhang, Zhang & Lu (2008); Zhang (2010); Zhang (2011a,b); Zhang (2012a,b).



Experimental

Crystal data

$[\text{Er}(\text{NO}_3)_2(\text{C}_6\text{H}_{18}\text{N}_3\text{OP})_4][\text{AgWS}_4]$	$V = 5299.8(17) \text{ \AA}^3$
$M_r = 1428.09$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 15.763(3) \text{ \AA}$	$\mu = 4.43 \text{ mm}^{-1}$
$b = 29.579(6) \text{ \AA}$	$T = 150 \text{ K}$
$c = 11.368(2) \text{ \AA}$	$0.2 \times 0.17 \times 0.15 \text{ mm}$
$\beta = 90.83(3)^\circ$	

Data collection

Rigaku Saturn724+ diffractometer	9597 independent reflections
Absorption correction: multi-scan	8722 reflections with $I > 2\sigma(I)$
(<i>CrystalClear</i> ; Rigaku, 2008)	$R_{\text{int}} = 0.044$
$T_{\text{min}} = 0.428$, $T_{\text{max}} = 0.514$	Standard reflections: 0
26753 measured reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$	532 parameters
$wR(F^2) = 0.092$	H-atom parameters constrained
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.91 \text{ e \AA}^{-3}$
9597 reflections	$\Delta\rho_{\text{min}} = -1.04 \text{ e \AA}^{-3}$

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5031).

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supporting information

Acta Cryst. (2013). E69, m43–m44 [https://doi.org/10.1107/S1600536812049987]

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S1. Comment

One-dimensional Mo(W)/S/Ag anionic polymers have attracted much attention for their configurational isomerism (Niu *et al.*, 2004; Zhang, Meng *et al.*, 2010) and unique properties as functional materials, such as third-order nonlinear optical (NLO) materials (Zhang, Song *et al.*, 2007). Different solvent-coordinated rare-earth cations proved effective to obtain various configurations of anionic chains (Niu *et al.*, 2004). The title compound, {[Er(hmp)₄(NO₃)₂][WS₄Ag]}_n (hmp = hexamethylphosphoramidate) with a wave-like anionic chain, was prepared by following such route using Er(III)-hmp complex as counterion.

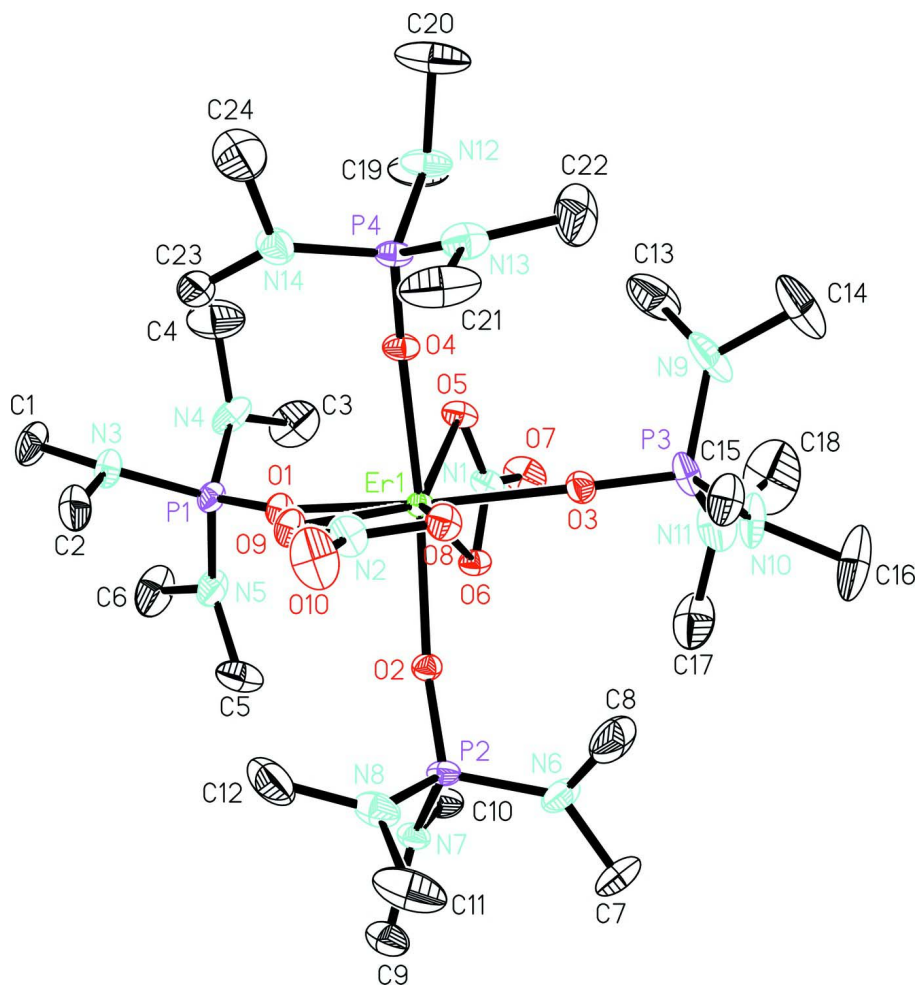
The title complex is isostructural with Y (Zhang, Cao *et al.*, 2007; Zhang, 2011*a*), Yb (Cao *et al.*, 2007), Eu (Zhang, Qian *et al.*, 2007), Nd (Tang, Zhang & Zhang, 2008), La (Tang, Zhang, Zhang & Lu, 2008), Dy (Zhang, 2010), Sm (Zhang, 2011*b*), Lu (Zhang, 2012*a*) and Tb (Zhang, 2012*b*) isomorphs. Er^{III} in the cation is coordinated by eight O atoms from two nitrate and four hmp ligands. In possession of two nitrate ligands, the cation in the title compound is univalent (Fig. 1), which leads to an anionic chain with a univalent repeat unit. As illustrated in Fig. 2, the anionic chain in the title compound has a distorted linear configuration with W—Ag—W and Ag—W—Ag angles of 161.37 (2) and 153.548 (12)°, respectively.

S2. Experimental

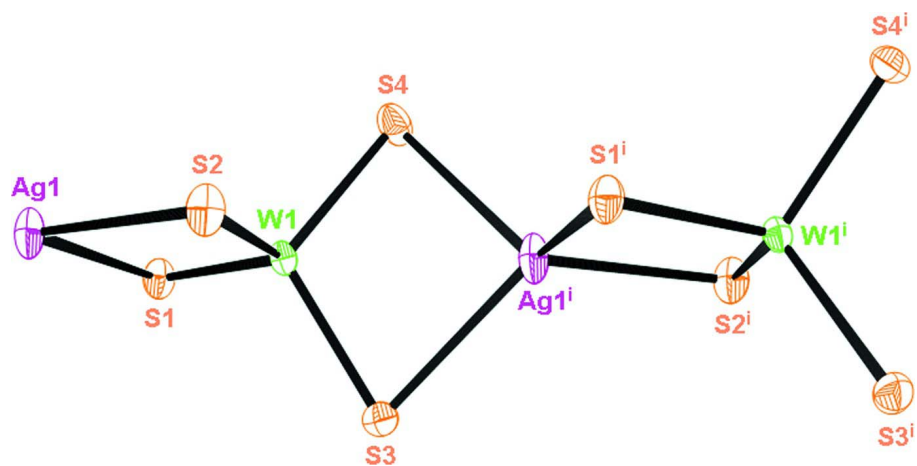
1 mmol AgI was added to a solution of [NH₄]₂WS₄ (1 mmol in 10 ml hmp) with thorough stirring for 30 minutes. The solution underwent an additional stir for two minute after 0.5 mmol Er(NO₃)₃·6H₂O was added. After filtration the orange filtrate was carefully laid on the surface with 15 ml *i*-PrOH. Orange block crystals were obtained after about one week.

S3. Refinement

H atoms were positioned geometrically and refined with riding model, with $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ and 0.96 Å for C—H bonds.

**Figure 1**

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

**Figure 2**

The molecular structure of a portion of the anionic chain in the title compound, with 30% probability displacement ellipsoids. Symmetry code: (i) $x, -y + 1/2, z + 1/2$.

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Crystal data

[Er(NO₃)₂(C₆H₁₈N₃OP)₄][AgWS₄]
 $M_r = 1428.09$
 Monoclinic, $P2_1/c$
 Hall symbol: -P 2ybc
 $a = 15.763$ (3) Å
 $b = 29.579$ (6) Å
 $c = 11.368$ (2) Å
 $\beta = 90.83$ (3)°
 $V = 5299.8$ (17) Å³
 $Z = 4$

$F(000) = 2828$
 $D_x = 1.790$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 16527 reflections
 $\theta = 3.2$ – 29.1 °
 $\mu = 4.43$ mm⁻¹
 $T = 150$ K
 Block, orange
 $0.2 \times 0.17 \times 0.15$ mm

Data collection

Rigaku Saturn724+
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2008)
 $T_{\min} = 0.428$, $T_{\max} = 0.514$

26753 measured reflections
 9597 independent reflections
 8722 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\text{max}} = 25.4$ °, $\theta_{\text{min}} = 3.2$ °
 $h = -15 \rightarrow 18$
 $k = -35 \rightarrow 33$
 $l = -13 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.092$
 $S = 1.08$
 9597 reflections
 532 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.024P)^2 + 26.5377P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.91$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.04$ e Å⁻³

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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Er1	0.261717 (18)	0.082599 (10)	0.17242 (3)	0.02182 (9)
P1	0.30083 (12)	-0.03020 (6)	0.29957 (18)	0.0304 (4)
P2	0.47743 (11)	0.13250 (6)	0.17898 (17)	0.0283 (4)

P3	0.20599 (14)	0.14671 (7)	-0.09571 (19)	0.0396 (5)
P4	0.04219 (11)	0.09630 (6)	0.26880 (18)	0.0301 (4)
O1	0.2929 (3)	0.01824 (14)	0.2704 (4)	0.0286 (11)
O2	0.3962 (3)	0.10679 (15)	0.1766 (4)	0.0270 (11)
O3	0.2272 (3)	0.12660 (16)	0.0203 (4)	0.0332 (12)
O4	0.1247 (3)	0.08070 (15)	0.2201 (5)	0.0314 (12)
O5	0.1983 (3)	0.02697 (16)	0.0365 (5)	0.0333 (12)
O6	0.3308 (3)	0.04094 (15)	0.0120 (4)	0.0309 (11)
O7	0.2627 (4)	0.00150 (19)	-0.1184 (5)	0.0517 (16)
O8	0.2475 (3)	0.15793 (16)	0.2617 (5)	0.0355 (12)
O9	0.2759 (3)	0.10278 (16)	0.3788 (4)	0.0326 (12)
O10	0.2730 (5)	0.1713 (2)	0.4458 (6)	0.0662 (19)
N1	0.2634 (4)	0.0222 (2)	-0.0254 (6)	0.0325 (14)
N2	0.2654 (4)	0.1450 (2)	0.3649 (6)	0.0387 (16)
N3	0.2788 (4)	-0.0367 (2)	0.4396 (5)	0.0369 (15)
N4	0.2357 (5)	-0.0654 (2)	0.2322 (6)	0.0455 (18)
N5	0.3945 (4)	-0.0479 (2)	0.2606 (6)	0.0471 (18)
N6	0.4773 (4)	0.1728 (2)	0.0807 (7)	0.0453 (18)
N7	0.5551 (3)	0.0976 (2)	0.1525 (5)	0.0321 (14)
N8	0.4928 (4)	0.1561 (3)	0.3049 (6)	0.0478 (18)
N9	0.1046 (5)	0.1388 (3)	-0.1233 (8)	0.072 (3)
N10	0.2258 (5)	0.2001 (2)	-0.0937 (6)	0.051 (2)
N11	0.2596 (6)	0.1239 (3)	-0.1975 (7)	0.063 (2)
N12	-0.0330 (4)	0.0706 (2)	0.1969 (6)	0.0448 (18)
N13	0.0175 (4)	0.1493 (2)	0.2613 (7)	0.0478 (18)
N14	0.0442 (4)	0.0864 (2)	0.4119 (6)	0.0444 (17)
C1	0.2737 (6)	-0.0824 (3)	0.4912 (8)	0.055 (2)
H1A	0.2610	-0.0801	0.5733	0.082*
H1B	0.3269	-0.0977	0.4821	0.082*
H1C	0.2297	-0.0993	0.4518	0.082*
C2	0.3022 (6)	-0.0022 (3)	0.5231 (8)	0.054 (2)
H2A	0.2852	-0.0113	0.6003	0.081*
H2B	0.2744	0.0256	0.5022	0.081*
H2C	0.3626	0.0021	0.5224	0.081*
C3	0.2467 (7)	-0.0811 (3)	0.1146 (10)	0.076 (3)
H3A	0.2009	-0.1011	0.0934	0.114*
H3B	0.2996	-0.0971	0.1096	0.114*
H3C	0.2471	-0.0558	0.0618	0.114*
C4	0.1460 (6)	-0.0679 (4)	0.2662 (11)	0.084 (4)
H4A	0.1171	-0.0898	0.2179	0.126*
H4B	0.1200	-0.0388	0.2554	0.126*
H4C	0.1426	-0.0766	0.3473	0.126*
C5	0.4648 (5)	-0.0170 (3)	0.2516 (9)	0.060 (3)
H5A	0.5145	-0.0333	0.2284	0.089*
H5B	0.4751	-0.0029	0.3265	0.089*
H5C	0.4516	0.0057	0.1939	0.089*
C6	0.4187 (7)	-0.0955 (3)	0.2793 (10)	0.077 (3)
H6A	0.4756	-0.1002	0.2528	0.115*

H6B	0.3805	-0.1148	0.2358	0.115*
H6C	0.4157	-0.1026	0.3615	0.115*
C7	0.5461 (6)	0.1830 (3)	0.0021 (9)	0.060 (3)
H7A	0.5306	0.2081	-0.0470	0.090*
H7B	0.5573	0.1571	-0.0462	0.090*
H7C	0.5960	0.1904	0.0474	0.090*
C8	0.4101 (6)	0.2069 (3)	0.0814 (10)	0.069 (3)
H8A	0.4190	0.2281	0.0189	0.103*
H8B	0.4111	0.2225	0.1555	0.103*
H8C	0.3561	0.1924	0.0703	0.103*
C9	0.6430 (5)	0.1065 (3)	0.1885 (8)	0.052 (2)
H9A	0.6784	0.0820	0.1639	0.078*
H9B	0.6464	0.1094	0.2726	0.078*
H9C	0.6619	0.1341	0.1528	0.078*
C10	0.5464 (5)	0.0644 (3)	0.0569 (7)	0.0403 (19)
H10A	0.5972	0.0466	0.0527	0.060*
H10B	0.5372	0.0799	-0.0164	0.060*
H10C	0.4989	0.0450	0.0719	0.060*
C11	0.5348 (6)	0.2001 (4)	0.3221 (10)	0.085 (4)
H11A	0.5376	0.2070	0.4045	0.127*
H11B	0.5031	0.2231	0.2814	0.127*
H11C	0.5912	0.1987	0.2915	0.127*
C12	0.4797 (6)	0.1309 (5)	0.4108 (9)	0.085 (4)
H12A	0.4919	0.1498	0.4777	0.127*
H12B	0.5167	0.1051	0.4123	0.127*
H12C	0.4218	0.1210	0.4133	0.127*
C13	0.0645 (7)	0.0960 (4)	-0.1105 (11)	0.082 (4)
H13A	0.0056	0.0985	-0.1321	0.124*
H13B	0.0695	0.0862	-0.0302	0.124*
H13C	0.0913	0.0743	-0.1606	0.124*
C14	0.0490 (8)	0.1713 (4)	-0.1835 (11)	0.099 (5)
H14A	-0.0070	0.1587	-0.1911	0.148*
H14B	0.0707	0.1777	-0.2601	0.148*
H14C	0.0467	0.1987	-0.1385	0.148*
C15	0.1981 (6)	0.2275 (3)	0.0056 (7)	0.049 (2)
H15A	0.2141	0.2584	-0.0068	0.073*
H15B	0.2244	0.2166	0.0768	0.073*
H15C	0.1375	0.2255	0.0120	0.073*
C16	0.2511 (9)	0.2258 (4)	-0.1981 (9)	0.092 (4)
H16A	0.2589	0.2570	-0.1773	0.137*
H16B	0.2077	0.2234	-0.2579	0.137*
H16C	0.3033	0.2138	-0.2275	0.137*
C17	0.3500 (7)	0.1209 (4)	-0.1868 (9)	0.078 (3)
H17A	0.3722	0.1064	-0.2554	0.116*
H17B	0.3648	0.1035	-0.1183	0.116*
H17C	0.3735	0.1507	-0.1796	0.116*
C18	0.2210 (11)	0.1070 (5)	-0.3088 (9)	0.127 (6)
H18A	0.2645	0.0948	-0.3577	0.190*

H18B	0.1932	0.1315	-0.3492	0.190*
H18C	0.1803	0.0839	-0.2916	0.190*
C19	-0.0203 (5)	0.0279 (3)	0.1385 (10)	0.067 (3)
H19A	-0.0725	0.0184	0.1013	0.100*
H19B	-0.0028	0.0056	0.1953	0.100*
H19C	0.0227	0.0311	0.0803	0.100*
C20	-0.1227 (5)	0.0803 (4)	0.2196 (11)	0.084 (4)
H20A	-0.1578	0.0618	0.1693	0.126*
H20B	-0.1341	0.1116	0.2040	0.126*
H20C	-0.1347	0.0737	0.3003	0.126*
C21	0.0485 (6)	0.1832 (3)	0.3428 (12)	0.085 (4)
H21A	0.0259	0.2122	0.3211	0.127*
H21B	0.1093	0.1842	0.3405	0.127*
H21C	0.0309	0.1757	0.4209	0.127*
C22	-0.0138 (8)	0.1691 (4)	0.1509 (10)	0.092 (4)
H22A	-0.0252	0.2007	0.1623	0.138*
H22B	-0.0651	0.1540	0.1266	0.138*
H22C	0.0282	0.1655	0.0913	0.138*
C23	0.0923 (5)	0.0480 (3)	0.4562 (8)	0.053 (2)
H23A	0.0877	0.0466	0.5403	0.079*
H23B	0.1509	0.0514	0.4358	0.079*
H23C	0.0703	0.0207	0.4220	0.079*
C24	-0.0291 (7)	0.0965 (4)	0.4838 (9)	0.085 (4)
H24A	-0.0169	0.0887	0.5642	0.127*
H24B	-0.0771	0.0794	0.4559	0.127*
H24C	-0.0418	0.1282	0.4787	0.127*
W1	0.783523 (17)	0.227488 (9)	0.52651 (2)	0.02184 (8)
Ag1	0.78222 (4)	0.26566 (2)	0.28700 (5)	0.03871 (16)
S1	0.78533 (12)	0.18464 (6)	0.36793 (16)	0.0312 (4)
S2	0.78321 (13)	0.30066 (6)	0.48679 (17)	0.0361 (5)
S3	0.66880 (12)	0.21148 (7)	0.62708 (17)	0.0353 (4)
S4	0.89701 (12)	0.21219 (7)	0.63272 (17)	0.0382 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.01984 (16)	0.01636 (16)	0.02925 (18)	0.00031 (11)	0.00027 (13)	0.00062 (13)
P1	0.0344 (10)	0.0222 (10)	0.0347 (11)	0.0047 (8)	0.0069 (9)	0.0060 (8)
P2	0.0217 (9)	0.0340 (11)	0.0293 (10)	-0.0055 (8)	-0.0002 (8)	-0.0064 (8)
P3	0.0588 (14)	0.0271 (11)	0.0324 (11)	0.0096 (9)	-0.0183 (10)	-0.0012 (9)
P4	0.0204 (9)	0.0275 (10)	0.0425 (12)	0.0011 (7)	0.0024 (8)	-0.0075 (9)
O1	0.037 (3)	0.016 (2)	0.033 (3)	0.003 (2)	0.001 (2)	0.002 (2)
O2	0.023 (2)	0.025 (3)	0.033 (3)	0.0008 (19)	0.001 (2)	0.001 (2)
O3	0.033 (3)	0.030 (3)	0.036 (3)	0.000 (2)	-0.005 (2)	0.005 (2)
O4	0.023 (2)	0.026 (3)	0.045 (3)	0.003 (2)	0.004 (2)	-0.004 (2)
O5	0.026 (3)	0.026 (3)	0.048 (3)	0.002 (2)	-0.004 (2)	-0.007 (2)
O6	0.024 (3)	0.028 (3)	0.040 (3)	0.000 (2)	0.003 (2)	-0.002 (2)
O7	0.056 (4)	0.051 (4)	0.048 (4)	0.004 (3)	-0.005 (3)	-0.026 (3)

O8	0.038 (3)	0.025 (3)	0.043 (3)	0.004 (2)	-0.001 (3)	0.000 (2)
O9	0.044 (3)	0.023 (3)	0.032 (3)	0.001 (2)	0.005 (2)	0.001 (2)
O10	0.100 (5)	0.045 (4)	0.053 (4)	0.018 (4)	-0.009 (4)	-0.020 (3)
N1	0.027 (3)	0.031 (3)	0.039 (4)	0.003 (3)	-0.005 (3)	-0.007 (3)
N2	0.047 (4)	0.029 (4)	0.040 (4)	0.005 (3)	-0.001 (3)	-0.009 (3)
N3	0.052 (4)	0.029 (3)	0.030 (4)	0.005 (3)	0.006 (3)	0.005 (3)
N4	0.059 (5)	0.025 (3)	0.054 (5)	-0.009 (3)	0.024 (4)	-0.007 (3)
N5	0.043 (4)	0.043 (4)	0.056 (5)	0.019 (3)	0.015 (3)	0.021 (4)
N6	0.037 (4)	0.036 (4)	0.064 (5)	-0.004 (3)	0.014 (3)	0.013 (3)
N7	0.020 (3)	0.045 (4)	0.031 (3)	0.001 (3)	0.001 (3)	-0.003 (3)
N8	0.036 (4)	0.069 (5)	0.039 (4)	0.000 (3)	-0.003 (3)	-0.022 (4)
N9	0.072 (6)	0.043 (5)	0.101 (7)	0.019 (4)	-0.055 (5)	0.000 (5)
N10	0.092 (6)	0.030 (4)	0.033 (4)	0.012 (4)	0.002 (4)	0.011 (3)
N11	0.092 (6)	0.049 (5)	0.049 (5)	0.025 (4)	0.003 (5)	-0.009 (4)
N12	0.023 (3)	0.053 (4)	0.058 (5)	0.000 (3)	0.006 (3)	-0.032 (4)
N13	0.039 (4)	0.034 (4)	0.070 (5)	0.003 (3)	0.009 (4)	-0.010 (4)
N14	0.037 (4)	0.058 (5)	0.038 (4)	0.010 (3)	0.000 (3)	-0.004 (3)
C1	0.067 (6)	0.040 (5)	0.057 (6)	0.015 (4)	0.020 (5)	0.024 (4)
C2	0.067 (6)	0.053 (6)	0.042 (5)	0.009 (5)	-0.001 (5)	0.013 (5)
C3	0.097 (8)	0.055 (6)	0.077 (8)	-0.023 (6)	0.010 (7)	-0.030 (6)
C4	0.062 (7)	0.086 (8)	0.104 (10)	-0.018 (6)	0.003 (7)	-0.033 (7)
C5	0.034 (5)	0.059 (6)	0.086 (8)	0.003 (4)	-0.010 (5)	-0.008 (6)
C6	0.091 (8)	0.057 (6)	0.083 (8)	0.038 (6)	0.035 (6)	0.025 (6)
C7	0.060 (6)	0.049 (6)	0.072 (7)	-0.021 (5)	0.026 (5)	0.008 (5)
C8	0.069 (7)	0.035 (5)	0.103 (9)	-0.004 (5)	0.018 (6)	0.022 (5)
C9	0.034 (5)	0.072 (6)	0.050 (6)	0.005 (4)	-0.004 (4)	-0.011 (5)
C10	0.030 (4)	0.054 (5)	0.036 (5)	-0.002 (4)	0.010 (3)	-0.013 (4)
C11	0.061 (7)	0.091 (8)	0.102 (9)	-0.002 (6)	-0.024 (6)	-0.070 (8)
C12	0.052 (6)	0.160 (12)	0.043 (6)	0.016 (7)	-0.011 (5)	-0.003 (7)
C13	0.068 (7)	0.062 (7)	0.116 (10)	0.001 (6)	-0.045 (7)	-0.012 (7)
C14	0.111 (10)	0.074 (8)	0.108 (10)	0.036 (7)	-0.065 (8)	-0.002 (7)
C15	0.077 (6)	0.026 (4)	0.043 (5)	0.009 (4)	0.010 (5)	-0.001 (4)
C16	0.172 (13)	0.057 (7)	0.047 (7)	0.024 (7)	0.034 (7)	0.022 (5)
C17	0.100 (9)	0.075 (7)	0.059 (7)	0.034 (7)	0.035 (6)	0.008 (6)
C18	0.217 (17)	0.130 (12)	0.034 (6)	-0.022 (12)	0.002 (8)	-0.046 (7)
C19	0.035 (5)	0.064 (6)	0.101 (9)	-0.005 (4)	0.005 (5)	-0.042 (6)
C20	0.029 (5)	0.110 (9)	0.114 (10)	0.001 (5)	0.003 (5)	-0.076 (8)
C21	0.052 (6)	0.037 (5)	0.165 (13)	-0.011 (4)	0.029 (7)	-0.049 (7)
C22	0.103 (9)	0.083 (8)	0.091 (9)	0.058 (7)	0.031 (7)	0.037 (7)
C23	0.040 (5)	0.078 (7)	0.040 (5)	-0.002 (5)	0.002 (4)	0.005 (5)
C24	0.069 (7)	0.128 (10)	0.058 (7)	0.045 (7)	0.019 (6)	-0.012 (7)
W1	0.02715 (16)	0.02019 (15)	0.01811 (15)	0.00253 (11)	-0.00214 (11)	-0.00094 (11)
Ag1	0.0607 (4)	0.0356 (3)	0.0198 (3)	0.0003 (3)	-0.0010 (3)	0.0023 (2)
S1	0.0455 (11)	0.0234 (9)	0.0246 (9)	-0.0004 (8)	0.0008 (8)	-0.0048 (7)
S2	0.0564 (13)	0.0218 (9)	0.0301 (10)	0.0037 (8)	0.0015 (9)	-0.0032 (8)
S3	0.0301 (10)	0.0457 (12)	0.0301 (10)	-0.0059 (8)	0.0016 (8)	-0.0020 (9)
S4	0.0353 (11)	0.0491 (12)	0.0300 (10)	0.0155 (9)	-0.0064 (9)	-0.0044 (9)

Geometric parameters (Å, °)

Er1—O3	2.225 (5)	C6—H6A	0.9600
Er1—O4	2.235 (5)	C6—H6B	0.9600
Er1—O2	2.237 (4)	C6—H6C	0.9600
Er1—O1	2.256 (4)	C7—H7A	0.9600
Er1—O9	2.428 (5)	C7—H7B	0.9600
Er1—O5	2.460 (5)	C7—H7C	0.9600
Er1—O8	2.460 (5)	C8—H8A	0.9600
Er1—O6	2.468 (5)	C8—H8B	0.9600
Er1—N2	2.863 (6)	C8—H8C	0.9600
Er1—N1	2.872 (6)	C9—H9A	0.9600
P1—O1	1.476 (5)	C9—H9B	0.9600
P1—N5	1.634 (7)	C9—H9C	0.9600
P1—N4	1.644 (7)	C10—H10A	0.9600
P1—N3	1.646 (6)	C10—H10B	0.9600
P2—O2	1.489 (5)	C10—H10C	0.9600
P2—N8	1.609 (7)	C11—H11A	0.9600
P2—N7	1.634 (6)	C11—H11B	0.9600
P2—N6	1.633 (7)	C11—H11C	0.9600
P3—O3	1.481 (5)	C12—H12A	0.9600
P3—N11	1.593 (8)	C12—H12B	0.9600
P3—N10	1.610 (7)	C12—H12C	0.9600
P3—N9	1.640 (8)	C13—H13A	0.9600
P4—O4	1.494 (5)	C13—H13B	0.9600
P4—N13	1.619 (7)	C13—H13C	0.9600
P4—N12	1.620 (6)	C14—H14A	0.9600
P4—N14	1.653 (7)	C14—H14B	0.9600
O5—N1	1.260 (8)	C14—H14C	0.9600
O6—N1	1.266 (7)	C15—H15A	0.9600
O7—N1	1.223 (8)	C15—H15B	0.9600
O8—N2	1.262 (8)	C15—H15C	0.9600
O9—N2	1.269 (8)	C16—H16A	0.9600
O10—N2	1.208 (8)	C16—H16B	0.9600
N3—C2	1.438 (10)	C16—H16C	0.9600
N3—C1	1.476 (9)	C17—H17A	0.9600
N4—C3	1.429 (12)	C17—H17B	0.9600
N4—C4	1.472 (12)	C17—H17C	0.9600
N5—C5	1.442 (11)	C18—H18A	0.9600
N5—C6	1.473 (11)	C18—H18B	0.9600
N6—C7	1.446 (10)	C18—H18C	0.9600
N6—C8	1.462 (11)	C19—H19A	0.9600
N7—C9	1.463 (9)	C19—H19B	0.9600
N7—C10	1.470 (9)	C19—H19C	0.9600
N8—C12	1.433 (13)	C20—H20A	0.9600
N8—C11	1.470 (12)	C20—H20B	0.9600
N9—C13	1.425 (12)	C20—H20C	0.9600
N9—C14	1.464 (11)	C21—H21A	0.9600

N10—C15	1.461 (10)	C21—H21B	0.9600
N10—C16	1.471 (11)	C21—H21C	0.9600
N11—C17	1.430 (13)	C22—H22A	0.9600
N11—C18	1.482 (12)	C22—H22B	0.9600
N12—C19	1.444 (10)	C22—H22C	0.9600
N12—C20	1.468 (10)	C23—H23A	0.9600
N13—C21	1.445 (11)	C23—H23B	0.9600
N13—C22	1.463 (12)	C23—H23C	0.9600
N14—C23	1.450 (10)	C24—H24A	0.9600
N14—C24	1.457 (11)	C24—H24B	0.9600
C1—H1A	0.9600	C24—H24C	0.9600
C1—H1B	0.9600	W1—S4	2.1909 (19)
C1—H1C	0.9600	W1—S1	2.2043 (18)
C2—H2A	0.9600	W1—S3	2.205 (2)
C2—H2B	0.9600	W1—S2	2.2108 (19)
C2—H2C	0.9600	W1—Ag1	2.9474 (8)
C3—H3A	0.9600	W1—Ag1 ⁱ	2.9685 (8)
C3—H3B	0.9600	Ag1—S2	2.496 (2)
C3—H3C	0.9600	Ag1—S1	2.5674 (19)
C4—H4A	0.9600	Ag1—S3 ⁱⁱ	2.620 (2)
C4—H4B	0.9600	Ag1—S4 ⁱⁱ	2.621 (2)
C4—H4C	0.9600	Ag1—W1 ⁱⁱ	2.9685 (8)
C5—H5A	0.9600	S3—Ag1 ⁱ	2.620 (2)
C5—H5B	0.9600	S4—Ag1 ⁱ	2.621 (2)
C5—H5C	0.9600		
O3—Er1—O4	88.67 (18)	N5—C5—H5C	109.5
O3—Er1—O2	92.88 (17)	H5A—C5—H5C	109.5
O4—Er1—O2	157.15 (17)	H5B—C5—H5C	109.5
O3—Er1—O1	157.85 (17)	N5—C6—H6A	109.5
O4—Er1—O1	93.63 (17)	N5—C6—H6B	109.5
O2—Er1—O1	93.44 (16)	H6A—C6—H6B	109.5
O3—Er1—O9	128.68 (17)	N5—C6—H6C	109.5
O4—Er1—O9	81.22 (17)	H6A—C6—H6C	109.5
O2—Er1—O9	80.05 (17)	H6B—C6—H6C	109.5
O1—Er1—O9	73.38 (16)	N6—C7—H7A	109.5
O3—Er1—O5	79.08 (17)	N6—C7—H7B	109.5
O4—Er1—O5	75.53 (17)	H7A—C7—H7B	109.5
O2—Er1—O5	127.14 (17)	N6—C7—H7C	109.5
O1—Er1—O5	80.18 (16)	H7A—C7—H7C	109.5
O9—Er1—O5	143.35 (17)	H7B—C7—H7C	109.5
O3—Er1—O8	76.60 (18)	N6—C8—H8A	109.5
O4—Er1—O8	80.12 (17)	N6—C8—H8B	109.5
O2—Er1—O8	78.09 (16)	H8A—C8—H8B	109.5
O1—Er1—O8	125.51 (17)	N6—C8—H8C	109.5
O9—Er1—O8	52.13 (16)	H8A—C8—H8C	109.5
O5—Er1—O8	145.74 (16)	H8B—C8—H8C	109.5
O3—Er1—O6	79.83 (17)	N7—C9—H9A	109.5

O4—Er1—O6	127.23 (16)	N7—C9—H9B	109.5
O2—Er1—O6	75.36 (16)	H9A—C9—H9B	109.5
O1—Er1—O6	81.28 (16)	N7—C9—H9C	109.5
O9—Er1—O6	143.29 (16)	H9A—C9—H9C	109.5
O5—Er1—O6	51.78 (16)	H9B—C9—H9C	109.5
O8—Er1—O6	143.25 (17)	N7—C10—H10A	109.5
O3—Er1—N2	102.64 (19)	N7—C10—H10B	109.5
O4—Er1—N2	80.79 (18)	H10A—C10—H10B	109.5
O2—Er1—N2	76.62 (18)	N7—C10—H10C	109.5
O1—Er1—N2	99.48 (18)	H10A—C10—H10C	109.5
O9—Er1—N2	26.14 (17)	H10B—C10—H10C	109.5
O5—Er1—N2	156.23 (18)	N8—C11—H11A	109.5
O8—Er1—N2	26.05 (17)	N8—C11—H11B	109.5
O6—Er1—N2	151.96 (17)	H11A—C11—H11B	109.5
O3—Er1—N1	76.12 (18)	N8—C11—H11C	109.5
O4—Er1—N1	101.18 (17)	H11A—C11—H11C	109.5
O2—Er1—N1	101.32 (17)	H11B—C11—H11C	109.5
O1—Er1—N1	81.82 (17)	N8—C12—H12A	109.5
O9—Er1—N1	155.20 (16)	N8—C12—H12B	109.5
O5—Er1—N1	25.89 (16)	H12A—C12—H12B	109.5
O8—Er1—N1	152.64 (18)	N8—C12—H12C	109.5
O6—Er1—N1	26.06 (15)	H12A—C12—H12C	109.5
N2—Er1—N1	177.59 (19)	H12B—C12—H12C	109.5
O1—P1—N5	109.0 (3)	N9—C13—H13A	109.5
O1—P1—N4	117.4 (3)	N9—C13—H13B	109.5
N5—P1—N4	103.4 (4)	H13A—C13—H13B	109.5
O1—P1—N3	108.2 (3)	N9—C13—H13C	109.5
N5—P1—N3	115.4 (3)	H13A—C13—H13C	109.5
N4—P1—N3	103.7 (3)	H13B—C13—H13C	109.5
O2—P2—N8	110.9 (3)	N9—C14—H14A	109.5
O2—P2—N7	108.7 (3)	N9—C14—H14B	109.5
N8—P2—N7	109.6 (3)	H14A—C14—H14B	109.5
O2—P2—N6	111.6 (3)	N9—C14—H14C	109.5
N8—P2—N6	106.9 (4)	H14A—C14—H14C	109.5
N7—P2—N6	109.2 (3)	H14B—C14—H14C	109.5
O3—P3—N11	111.2 (4)	N10—C15—H15A	109.5
O3—P3—N10	109.9 (3)	N10—C15—H15B	109.5
N11—P3—N10	108.8 (4)	H15A—C15—H15B	109.5
O3—P3—N9	108.7 (4)	N10—C15—H15C	109.5
N11—P3—N9	109.0 (5)	H15A—C15—H15C	109.5
N10—P3—N9	109.3 (4)	H15B—C15—H15C	109.5
O4—P4—N13	119.4 (3)	N10—C16—H16A	109.5
O4—P4—N12	107.6 (3)	N10—C16—H16B	109.5
N13—P4—N12	104.7 (4)	H16A—C16—H16B	109.5
O4—P4—N14	107.8 (3)	N10—C16—H16C	109.5
N13—P4—N14	103.0 (4)	H16A—C16—H16C	109.5
N12—P4—N14	114.7 (4)	H16B—C16—H16C	109.5
P1—O1—Er1	161.3 (3)	N11—C17—H17A	109.5

P2—O2—Er1	168.0 (3)	N11—C17—H17B	109.5
P3—O3—Er1	167.6 (3)	H17A—C17—H17B	109.5
P4—O4—Er1	158.7 (3)	N11—C17—H17C	109.5
N1—O5—Er1	95.6 (4)	H17A—C17—H17C	109.5
N1—O6—Er1	95.1 (4)	H17B—C17—H17C	109.5
N2—O8—Er1	95.1 (4)	N11—C18—H18A	109.5
N2—O9—Er1	96.4 (4)	N11—C18—H18B	109.5
O7—N1—O5	122.8 (6)	H18A—C18—H18B	109.5
O7—N1—O6	120.4 (6)	N11—C18—H18C	109.5
O5—N1—O6	116.8 (6)	H18A—C18—H18C	109.5
O7—N1—Er1	171.6 (5)	H18B—C18—H18C	109.5
O5—N1—Er1	58.5 (3)	N12—C19—H19A	109.5
O6—N1—Er1	58.9 (3)	N12—C19—H19B	109.5
O10—N2—O8	122.1 (7)	H19A—C19—H19B	109.5
O10—N2—O9	121.8 (7)	N12—C19—H19C	109.5
O8—N2—O9	116.1 (6)	H19A—C19—H19C	109.5
O10—N2—Er1	175.5 (6)	H19B—C19—H19C	109.5
O8—N2—Er1	58.9 (3)	N12—C20—H20A	109.5
O9—N2—Er1	57.4 (3)	N12—C20—H20B	109.5
C2—N3—C1	113.8 (7)	H20A—C20—H20B	109.5
C2—N3—P1	120.0 (5)	N12—C20—H20C	109.5
C1—N3—P1	120.3 (5)	H20A—C20—H20C	109.5
C3—N4—C4	111.1 (8)	H20B—C20—H20C	109.5
C3—N4—P1	123.9 (6)	N13—C21—H21A	109.5
C4—N4—P1	120.3 (6)	N13—C21—H21B	109.5
C5—N5—C6	114.7 (7)	H21A—C21—H21B	109.5
C5—N5—P1	120.9 (6)	N13—C21—H21C	109.5
C6—N5—P1	120.1 (6)	H21A—C21—H21C	109.5
C7—N6—C8	114.2 (7)	H21B—C21—H21C	109.5
C7—N6—P2	125.5 (6)	N13—C22—H22A	109.5
C8—N6—P2	119.5 (6)	N13—C22—H22B	109.5
C9—N7—C10	114.0 (6)	H22A—C22—H22B	109.5
C9—N7—P2	122.9 (5)	N13—C22—H22C	109.5
C10—N7—P2	119.7 (5)	H22A—C22—H22C	109.5
C12—N8—C11	114.8 (8)	H22B—C22—H22C	109.5
C12—N8—P2	120.0 (7)	N14—C23—H23A	109.5
C11—N8—P2	124.3 (7)	N14—C23—H23B	109.5
C13—N9—C14	111.5 (8)	H23A—C23—H23B	109.5
C13—N9—P3	122.7 (6)	N14—C23—H23C	109.5
C14—N9—P3	124.9 (8)	H23A—C23—H23C	109.5
C15—N10—C16	115.1 (7)	H23B—C23—H23C	109.5
C15—N10—P3	119.7 (6)	N14—C24—H24A	109.5
C16—N10—P3	123.4 (7)	N14—C24—H24B	109.5
C17—N11—C18	116.6 (9)	H24A—C24—H24B	109.5
C17—N11—P3	120.2 (7)	N14—C24—H24C	109.5
C18—N11—P3	123.2 (9)	H24A—C24—H24C	109.5
C19—N12—C20	113.0 (6)	H24B—C24—H24C	109.5
C19—N12—P4	122.5 (5)	S4—W1—S1	108.17 (7)

C20—N12—P4	121.3 (5)	S4—W1—S3	109.83 (8)
C21—N13—C22	112.4 (8)	S1—W1—S3	108.72 (7)
C21—N13—P4	124.0 (7)	S4—W1—S2	108.30 (8)
C22—N13—P4	120.7 (7)	S1—W1—S2	113.32 (7)
C23—N14—C24	112.4 (8)	S3—W1—S2	108.46 (8)
C23—N14—P4	118.9 (6)	S4—W1—Ag1	125.65 (6)
C24—N14—P4	120.7 (6)	S1—W1—Ag1	57.64 (5)
N3—C1—H1A	109.5	S3—W1—Ag1	124.50 (6)
N3—C1—H1B	109.5	S2—W1—Ag1	55.69 (5)
H1A—C1—H1B	109.5	S4—W1—Ag1 ⁱ	58.79 (6)
N3—C1—H1C	109.5	S1—W1—Ag1 ⁱ	148.81 (5)
H1A—C1—H1C	109.5	S3—W1—Ag1 ⁱ	58.66 (5)
H1B—C1—H1C	109.5	S2—W1—Ag1 ⁱ	97.87 (5)
N3—C2—H2A	109.5	Ag1—W1—Ag1 ⁱ	153.548 (12)
N3—C2—H2B	109.5	S2—Ag1—S1	93.51 (6)
H2A—C2—H2B	109.5	S2—Ag1—S3 ⁱⁱ	121.31 (7)
N3—C2—H2C	109.5	S1—Ag1—S3 ⁱⁱ	119.92 (6)
H2A—C2—H2C	109.5	S2—Ag1—S4 ⁱⁱ	120.66 (7)
H2B—C2—H2C	109.5	S1—Ag1—S4 ⁱⁱ	117.59 (7)
N4—C3—H3A	109.5	S3 ⁱⁱ —Ag1—S4 ⁱⁱ	86.67 (6)
N4—C3—H3B	109.5	S2—Ag1—W1	47.03 (5)
H3A—C3—H3B	109.5	S1—Ag1—W1	46.49 (4)
N4—C3—H3C	109.5	S3 ⁱⁱ —Ag1—W1	137.34 (5)
H3A—C3—H3C	109.5	S4 ⁱⁱ —Ag1—W1	135.90 (5)
H3B—C3—H3C	109.5	S2—Ag1—W1 ⁱⁱ	151.57 (5)
N4—C4—H4A	109.5	S1—Ag1—W1 ⁱⁱ	114.89 (5)
N4—C4—H4B	109.5	S3 ⁱⁱ —Ag1—W1 ⁱⁱ	45.95 (5)
H4A—C4—H4B	109.5	S4 ⁱⁱ —Ag1—W1 ⁱⁱ	45.63 (4)
N4—C4—H4C	109.5	W1—Ag1—W1 ⁱⁱ	161.37 (2)
H4A—C4—H4C	109.5	W1—S1—Ag1	75.87 (6)
H4B—C4—H4C	109.5	W1—S2—Ag1	77.28 (6)
N5—C5—H5A	109.5	W1—S3—Ag1 ⁱ	75.39 (6)
N5—C5—H5B	109.5	W1—S4—Ag1 ⁱ	75.59 (6)
H5A—C5—H5B	109.5		

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