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catena-Poly[[[tetrakis(dimethylformamide-κO)-magnesium(II)]-μ-diphenylphosphato-$\kappa^2 O:O'$] trifluoromethanesulfonate]

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.119
Data-to-parameter ratio = 13.4

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

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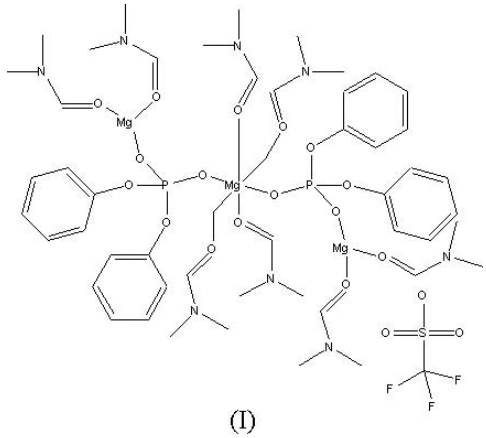
The title compound, $[Mg(C_{12}H_{10}O_4P)(C_3H_7NO)_4](CF_3O_3S)$, consists of diphenylphosphate anions linked into infinite chains by bridging magnesium ions, which are also coordinated by dimethylformamide molecules. A non-coordinated trifluoromethanesulfonate counter-ion provides charge balance. Both crystallographically distinct magnesium cations occupy special positions with $\overline{1}$ site symmetry.

Comment

There are few examples of phosphodiester molecules that are linked by magnesium ions (Cremlyn *et al.*, 1958; Ezra & Collin, 1973; Schwalbe *et al.*, 1973). Narayan *et al.* (1978) described an unusual crystal structure in which phosphodiester anions are linked by magnesium cations into a chain structure. This compound arose from the crystallization of magnesium diphenylphosphate in moist diethyl ether.



(I)

The related title compound, (I), arose from the attempted crystallization of an imidazole catalyst intermediate. The asymmeric unit of (I) (Fig. 1) contains one diphenylphosphate anion, four distinct dimethylformamide (DMF) molecules, one non-coordinated trifluoromethanesulfonate counter-ion and two crystallographically distinct octahedrally coordinated (Table 1) magnesium cations (both with site symmetry $\overline{1}$). The main differences between the structures are that (I) has DMF coordinated to Mg, whereas the Narayan *et al.* (1978) compound has water molecules. In the Narayan structure, four phosphate O atoms and two water molecules are coordinated to each Mg atom, whereas in (I), two phosphate O atoms and four DMF O atoms link to each Mg atom (Fig. 2). In the Narayan structure, the mean $Mg-O_P$ (P = phosphate) and $Mg-O_W$ (W = water) bond distances are 2.042 (4) and 2.154 (4) Å, respectively. Equivalent values of 2.0491 (18) and 2.075 (19) Å [for $Mg-O_D$ (D = DMF)] arise in (I). The

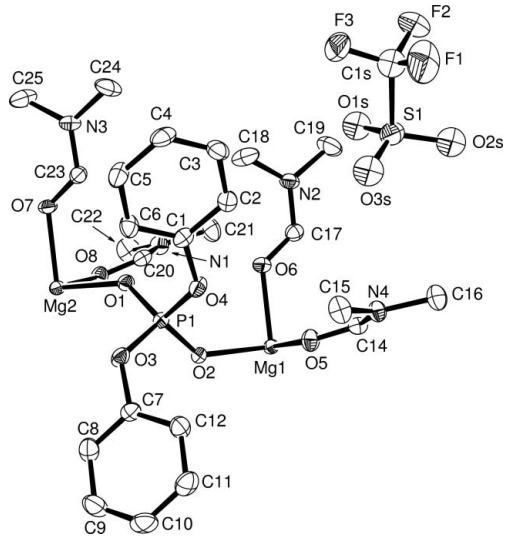


Figure 1
The asymmetic unit of (I), with displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity.

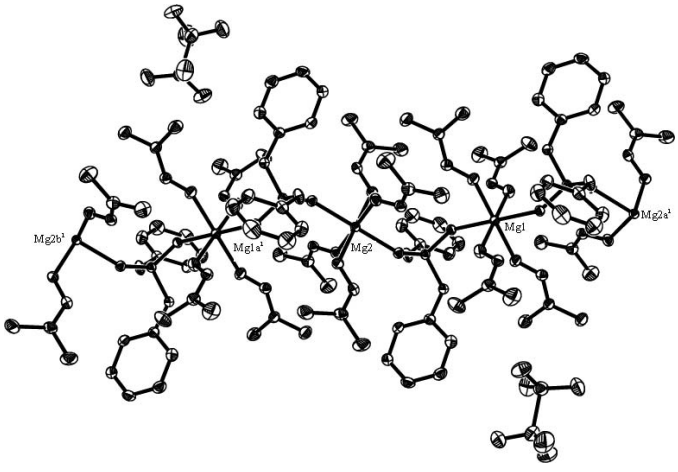


Figure 2
An extended view of the chain structure of (I) [symmetry code: (i) $-x, -y + 2, -z$]. H atoms have been omitted for clarity.

phosphorus–phenyl bond lengths are comparable in both structures. There appear to be no significant hydrogen-bonding intractions in (I).

Experimental

A solution of diphenyl chlorophosphate (0.319 g, 0.118 mmol), 2-{2-[2-(2-methoxyethoxy)ethoxy]ethoxymethyl}-1-methyl-1*H*-imidazole (0.25 g, 0.118 mmol), and magnesium trifluoromethanesulfonate (0.038 g, 0.118 mmol) in dry DMF (5 ml) in a specimen vial was submersed into a sealed specimen vial containing dry diethyl ether (5 ml). This was kept for 4 d at 283 K to allow slow growth of crystals. Once harvested, the crystals of (I) were very sensitive to atmospheric moisture and were prone decomposition whilst being handled.

Crystal data

$[Mg(C_{12}H_{10}O_4P)(C_3H_7NO)_4]$-$(CF_3O_3S)$	$Z = 2$
$M_r = 714.93$	$D_x = 1.427$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 11.2645$ (19) Å	Cell parameters from 139 reflections
$b = 11.4907$ (19) Å	$\theta = 7.3$–50.6°
$c = 13.665$ (2) Å	$\mu = 0.24$ mm^{-1}
$\alpha = 95.865$ (3)°	$T = 150$ (2) K
$\beta = 104.109$ (3)°	Block, colourless
$\gamma = 100.969$ (3)°	0.48 × 0.32 × 0.21 mm
$V = 1663.4$ (5) Å^3	

Data collection

Bruker SMART1000 CCD diffractometer	5729 independent reflections
ω scans	4183 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	$R_{int} = 0.035$
$T_{min} = 0.893$, $T_{max} = 0.951$	$\theta_{max} = 25.0^\circ$
11079 measured reflections	$h = -13 \rightarrow 12$
	$k = -13 \rightarrow 13$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 1.6348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.119$	$\Delta\rho_{max} = 0.63$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.46$ e Å^{-3}
5729 reflections	
426 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Mg1—O2	2.0532 (18)	Mg2—O1	2.0491 (18)
Mg1—O5	2.061 (2)	Mg2—O8	2.0695 (19)
Mg1—O6	2.0898 (18)	Mg2—O7	2.0808 (18)
P1—O1—Mg2	136.79 (11)	P1—O2—Mg1	136.67 (11)

H atoms were positioned geometrically, with C—H = 0.95–0.98 Å, and refined as riding (including torsional freedom for methyl groups) with the constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(methyl carrier).

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

EPSRC and Onyx Scientific for funding (AR).

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supporting information

Acta Cryst. (2005). E**61**, m1251–m1252 [https://doi.org/10.1107/S1600536805016880]

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Cell parameters from 139 reflections
$\theta = 7.3$–$50.6°$
$\mu = 0.24$ mm^{-1}
$T = 150$ K
Block, colourless
0.48 × 0.32 × 0.21 mm

Data collection

Bruker SMART1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 100 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1997)
$T_{min} = 0.893$, $T_{max} = 0.951$
11079 measured reflections
5729 independent reflections
4183 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -13 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.119$
$S = 1.01$
5729 reflections
426 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
$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 1.6348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ 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_{iso}*/U_{eq}
Mg1	0.5000	1.0000	0.0000	0.0163 (3)
Mg2	0.0000	1.0000	0.0000	0.0152 (3)
P1	0.21959 (7)	0.84881 (6)	−0.00364 (5)	0.01622 (18)
N1	0.2850 (2)	1.3132 (2)	0.13342 (18)	0.0238 (6)
N2	0.5530 (2)	1.0884 (2)	0.32025 (17)	0.0227 (6)
N3	0.0242 (2)	0.9762 (2)	0.31187 (17)	0.0246 (6)
N4	0.6733 (2)	0.7302 (2)	0.12015 (18)	0.0220 (5)
O1	0.14932 (17)	0.92208 (17)	0.04599 (13)	0.0182 (4)
O2	0.31636 (17)	0.90654 (17)	−0.05029 (13)	0.0172 (4)
O3	0.11520 (18)	0.74903 (18)	−0.08721 (14)	0.0237 (5)
O4	0.28850 (18)	0.77348 (18)	0.07570 (15)	0.0234 (5)
O5	0.55548 (18)	0.84476 (18)	0.03466 (15)	0.0243 (5)
O6	0.48216 (18)	1.03605 (18)	0.14812 (14)	0.0242 (5)
O7	−0.02261 (18)	1.00805 (18)	0.14702 (14)	0.0220 (5)
O8	0.11983 (18)	1.16805 (17)	0.04097 (15)	0.0230 (5)
C1	0.2471 (3)	0.7286 (3)	0.1559 (2)	0.0209 (6)
C2	0.3406 (3)	0.7238 (3)	0.2408 (2)	0.0235 (7)
H2	0.4262	0.7542	0.2438	0.028*
C3	0.3087 (3)	0.6741 (3)	0.3221 (2)	0.0290 (7)
H3	0.3725	0.6697	0.3807	0.035*
C4	0.1845 (3)	0.6314 (3)	0.3172 (2)	0.0305 (8)
H4	0.1625	0.5981	0.3729	0.037*
C5	0.0917 (3)	0.6365 (3)	0.2320 (2)	0.0306 (7)
H5	0.0061	0.6063	0.2292	0.037*
C6	0.1223 (3)	0.6859 (3)	0.1496 (2)	0.0261 (7)
H6	0.0585	0.6899	0.0908	0.031*
C7	0.1315 (3)	0.6921 (3)	−0.1765 (2)	0.0212 (6)
C8	0.0402 (3)	0.6878 (3)	−0.2651 (2)	0.0296 (7)
H8	−0.0276	0.7256	−0.2639	0.036*
C9	0.0474 (3)	0.6282 (3)	−0.3562 (2)	0.0373 (8)
H9	−0.0150	0.6255	−0.4178	0.045*
C10	0.1462 (3)	0.5727 (3)	−0.3568 (3)	0.0365 (8)
H10	0.1510	0.5310	−0.4189	0.044*
C11	0.2376 (3)	0.5779 (3)	−0.2674 (2)	0.0325 (8)
H11	0.3053	0.5398	−0.2683	0.039*

C12	0.2314 (3)	0.6384 (3)	−0.1764 (2)	0.0273 (7)
H12	0.2947	0.6428	−0.1149	0.033*
C14	0.6573 (3)	0.8306 (3)	0.0847 (2)	0.0209 (6)
H14	0.7284	0.8955	0.0986	0.025*
C15	0.5679 (3)	0.6296 (3)	0.1051 (3)	0.0315 (8)
H15A	0.4915	0.6493	0.0652	0.047*
H15B	0.5572	0.6125	0.1716	0.047*
H15C	0.5838	0.5589	0.0683	0.047*
C16	0.7970 (3)	0.7141 (3)	0.1727 (2)	0.0309 (7)
H16A	0.8116	0.6399	0.1405	0.046*
H16B	0.8011	0.7092	0.2446	0.046*
H16C	0.8615	0.7825	0.1685	0.046*
C17	0.5663 (3)	1.0837 (3)	0.2267 (2)	0.0217 (6)
H17	0.6461	1.1195	0.2190	0.026*
C18	0.4374 (3)	1.0288 (3)	0.3405 (2)	0.0373 (8)
H18A	0.3726	0.9994	0.2758	0.056*
H18B	0.4093	1.0858	0.3832	0.056*
H18C	0.4525	0.9611	0.3762	0.056*
C19	0.6576 (3)	1.1431 (3)	0.4093 (2)	0.0415 (9)
H19A	0.7307	1.1786	0.3868	0.062*
H19B	0.6784	1.0816	0.4511	0.062*
H19C	0.6338	1.2058	0.4497	0.062*
C20	0.2271 (3)	1.2007 (3)	0.0992 (2)	0.0218 (6)
H20	0.2704	1.1404	0.1204	0.026*
C21	0.4165 (3)	1.3460 (3)	0.1931 (3)	0.0362 (8)
H21A	0.4424	1.2747	0.2168	0.054*
H21B	0.4263	1.4066	0.2522	0.054*
H21C	0.4690	1.3788	0.1504	0.054*
C22	0.2233 (3)	1.4098 (3)	0.1063 (3)	0.0396 (9)
H22A	0.1335	1.3768	0.0749	0.059*
H22B	0.2603	1.4509	0.0577	0.059*
H22C	0.2345	1.4670	0.1679	0.059*
C23	0.0441 (3)	0.9752 (3)	0.2208 (2)	0.0205 (6)
H23	0.1151	0.9473	0.2109	0.025*
C24	0.1052 (3)	0.9325 (3)	0.3936 (2)	0.0367 (8)
H24A	0.1696	0.9025	0.3682	0.055*
H24B	0.0548	0.8673	0.4170	0.055*
H24C	0.1456	0.9981	0.4507	0.055*
C25	−0.0801 (3)	1.0216 (3)	0.3354 (2)	0.0371 (8)
H25A	−0.1301	1.0441	0.2738	0.056*
H25B	−0.0470	1.0922	0.3888	0.056*
H25C	−0.1332	0.9591	0.3593	0.056*
C1S	0.6746 (3)	0.6755 (4)	0.5500 (3)	0.0449 (10)
F1	0.7131 (2)	0.5738 (2)	0.5569 (2)	0.0771 (8)
F2	0.7410 (2)	0.7541 (3)	0.63436 (16)	0.0703 (8)
F3	0.5543 (2)	0.6534 (2)	0.55087 (17)	0.0600 (7)
S1	0.69565 (8)	0.73507 (8)	0.43589 (6)	0.0338 (2)
O1S	0.6450 (3)	0.8396 (2)	0.44028 (19)	0.0479 (7)

O2S	0.8287 (2)	0.7558 (2)	0.45062 (19)	0.0498 (7)
O3S	0.6225 (2)	0.6387 (2)	0.35533 (18)	0.0510 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0169 (7)	0.0185 (7)	0.0151 (6)	0.0057 (6)	0.0056 (5)	0.0033 (5)
Mg2	0.0165 (7)	0.0161 (7)	0.0142 (6)	0.0045 (5)	0.0054 (5)	0.0027 (5)
P1	0.0162 (4)	0.0167 (4)	0.0169 (4)	0.0045 (3)	0.0059 (3)	0.0025 (3)
N1	0.0253 (14)	0.0179 (14)	0.0260 (13)	0.0025 (11)	0.0059 (11)	0.0007 (11)
N2	0.0275 (14)	0.0255 (14)	0.0155 (12)	0.0080 (11)	0.0053 (10)	0.0015 (10)
N3	0.0315 (15)	0.0286 (15)	0.0150 (12)	0.0071 (12)	0.0085 (11)	0.0029 (11)
N4	0.0200 (13)	0.0210 (14)	0.0249 (13)	0.0054 (11)	0.0040 (10)	0.0055 (11)
O1	0.0190 (10)	0.0197 (11)	0.0175 (10)	0.0070 (8)	0.0058 (8)	0.0029 (8)
O2	0.0152 (10)	0.0202 (11)	0.0167 (10)	0.0035 (8)	0.0053 (8)	0.0032 (8)
O3	0.0192 (11)	0.0233 (11)	0.0266 (11)	0.0009 (9)	0.0096 (9)	−0.0060 (9)
O4	0.0215 (11)	0.0282 (12)	0.0284 (11)	0.0119 (9)	0.0128 (9)	0.0137 (9)
O5	0.0217 (11)	0.0229 (12)	0.0298 (11)	0.0082 (9)	0.0058 (9)	0.0070 (9)
O6	0.0224 (11)	0.0325 (12)	0.0160 (10)	0.0043 (9)	0.0053 (9)	−0.0004 (9)
O7	0.0252 (11)	0.0310 (12)	0.0146 (10)	0.0116 (9)	0.0089 (8)	0.0065 (9)
O8	0.0198 (11)	0.0197 (11)	0.0289 (11)	0.0019 (9)	0.0077 (9)	0.0032 (9)
C1	0.0257 (16)	0.0153 (15)	0.0263 (16)	0.0083 (12)	0.0122 (13)	0.0051 (12)
C2	0.0224 (16)	0.0207 (16)	0.0262 (16)	0.0042 (13)	0.0059 (13)	0.0005 (13)
C3	0.0319 (18)	0.0358 (19)	0.0203 (16)	0.0138 (15)	0.0034 (13)	0.0064 (14)
C4	0.040 (2)	0.0343 (19)	0.0284 (17)	0.0157 (16)	0.0202 (15)	0.0157 (14)
C5	0.0243 (17)	0.0345 (19)	0.0409 (19)	0.0118 (15)	0.0148 (15)	0.0181 (15)
C6	0.0220 (16)	0.0276 (18)	0.0312 (17)	0.0095 (14)	0.0058 (13)	0.0125 (14)
C7	0.0236 (16)	0.0155 (15)	0.0235 (15)	0.0012 (12)	0.0088 (13)	−0.0020 (12)
C8	0.0240 (17)	0.0283 (18)	0.0346 (18)	0.0067 (14)	0.0052 (14)	0.0016 (14)
C9	0.037 (2)	0.042 (2)	0.0247 (17)	0.0022 (17)	0.0000 (15)	−0.0028 (15)
C10	0.043 (2)	0.032 (2)	0.0292 (18)	−0.0007 (16)	0.0130 (16)	−0.0111 (15)
C11	0.0338 (19)	0.0275 (19)	0.0394 (19)	0.0124 (15)	0.0145 (15)	−0.0009 (15)
C12	0.0262 (17)	0.0265 (18)	0.0276 (17)	0.0082 (14)	0.0042 (13)	0.0007 (13)
C14	0.0238 (16)	0.0205 (16)	0.0192 (15)	0.0055 (13)	0.0074 (13)	0.0027 (12)
C15	0.0296 (18)	0.0218 (17)	0.0396 (19)	0.0042 (14)	0.0033 (15)	0.0067 (14)
C16	0.0258 (17)	0.0316 (19)	0.0350 (18)	0.0097 (14)	0.0034 (14)	0.0092 (15)
C17	0.0236 (16)	0.0213 (16)	0.0220 (16)	0.0064 (13)	0.0080 (13)	0.0047 (12)
C18	0.048 (2)	0.039 (2)	0.0293 (18)	0.0044 (17)	0.0225 (16)	0.0016 (15)
C19	0.045 (2)	0.053 (2)	0.0208 (17)	0.0132 (18)	−0.0003 (15)	−0.0022 (16)
C20	0.0250 (17)	0.0224 (17)	0.0217 (15)	0.0075 (13)	0.0113 (13)	0.0046 (12)
C21	0.0285 (18)	0.031 (2)	0.0396 (19)	−0.0027 (15)	−0.0005 (15)	0.0040 (15)
C22	0.047 (2)	0.0206 (18)	0.046 (2)	0.0083 (16)	0.0056 (17)	0.0002 (15)
C23	0.0192 (15)	0.0214 (16)	0.0205 (15)	0.0027 (12)	0.0072 (12)	0.0010 (12)
C24	0.047 (2)	0.046 (2)	0.0174 (16)	0.0139 (17)	0.0040 (15)	0.0097 (15)
C25	0.051 (2)	0.043 (2)	0.0294 (18)	0.0195 (18)	0.0240 (16)	0.0107 (16)
C1S	0.036 (2)	0.060 (3)	0.046 (2)	0.0209 (19)	0.0115 (18)	0.023 (2)
F1	0.0706 (17)	0.0762 (18)	0.112 (2)	0.0408 (15)	0.0338 (16)	0.0682 (17)
F2	0.0594 (16)	0.115 (2)	0.0293 (12)	0.0205 (15)	0.0012 (11)	0.0049 (13)

F3	0.0386 (13)	0.0981 (19)	0.0565 (14)	0.0200 (12)	0.0239 (11)	0.0357 (13)
S1	0.0374 (5)	0.0356 (5)	0.0331 (5)	0.0128 (4)	0.0134 (4)	0.0088 (4)
O1S	0.0636 (18)	0.0350 (15)	0.0484 (15)	0.0221 (13)	0.0110 (13)	0.0112 (12)
O2S	0.0326 (14)	0.0682 (19)	0.0527 (16)	0.0072 (13)	0.0196 (12)	0.0157 (14)
O3S	0.0518 (17)	0.0576 (18)	0.0367 (14)	0.0139 (14)	0.0071 (12)	−0.0148 (13)

Geometric parameters (Å, º)

Mg1—O2^{i}	2.0532 (18)	C7—C12	1.383 (4)
Mg1—O2	2.0532 (18)	C8—C9	1.386 (4)
Mg1—O5^{i}	2.061 (2)	C8—H8	0.9500
Mg1—O5	2.061 (2)	C9—C10	1.384 (5)
Mg1—O6^{i}	2.0898 (18)	C9—H9	0.9500
Mg1—O6	2.0898 (18)	C10—C11	1.381 (5)
Mg2—O1^{ii}	2.0491 (18)	C10—H10	0.9500
Mg2—O1	2.0491 (18)	C11—C12	1.385 (4)
Mg2—O8	2.0695 (19)	C11—H11	0.9500
Mg2—O8^{ii}	2.0695 (19)	C12—H12	0.9500
Mg2—O7	2.0808 (18)	C14—H14	0.9500
Mg2—O7^{ii}	2.0808 (18)	C15—H15A	0.9800
P1—O2	1.4780 (19)	C15—H15B	0.9800
P1—O1	1.4812 (19)	C15—H15C	0.9800
P1—O4	1.601 (2)	C16—H16A	0.9800
P1—O3	1.602 (2)	C16—H16B	0.9800
N1—C20	1.312 (4)	C16—H16C	0.9800
N1—C22	1.451 (4)	C17—H17	0.9500
N1—C21	1.463 (4)	C18—H18A	0.9800
N2—C17	1.319 (4)	C18—H18B	0.9800
N2—C18	1.455 (4)	C18—H18C	0.9800
N2—C19	1.458 (4)	C19—H19A	0.9800
N3—C23	1.316 (4)	C19—H19B	0.9800
N3—C24	1.458 (4)	C19—H19C	0.9800
N3—C25	1.463 (4)	C20—H20	0.9500
N4—C14	1.322 (4)	C21—H21A	0.9800
N4—C15	1.448 (4)	C21—H21B	0.9800
N4—C16	1.460 (4)	C21—H21C	0.9800
O3—C7	1.394 (3)	C22—H22A	0.9800
O4—C1	1.399 (3)	C22—H22B	0.9800
O5—C14	1.234 (3)	C22—H22C	0.9800
O6—C17	1.240 (3)	C23—H23	0.9500
O7—C23	1.241 (3)	C24—H24A	0.9800
O8—C20	1.238 (3)	C24—H24B	0.9800
C1—C6	1.377 (4)	C24—H24C	0.9800
C1—C2	1.377 (4)	C25—H25A	0.9800
C2—C3	1.391 (4)	C25—H25B	0.9800
C2—H2	0.9500	C25—H25C	0.9800
C3—C4	1.375 (4)	C1S—F1	1.326 (4)
C3—H3	0.9500	C1S—F3	1.333 (4)

C4—C5	1.377 (4)	C1S—F2	1.347 (4)
C4—H4	0.9500	C1S—S1	1.815 (4)
C5—C6	1.397 (4)	S1—O1S	1.426 (2)
C5—H5	0.9500	S1—O2S	1.432 (3)
C6—H6	0.9500	S1—O3S	1.442 (3)
C7—C8	1.374 (4)		

O2^{i}—Mg1—O2	180.0	C8—C9—H9	120.2
O2^{i}—Mg1—O5^{i}	90.09 (8)	C11—C10—C9	120.2 (3)
O2—Mg1—O5^{i}	89.91 (8)	C11—C10—H10	119.9
O2^{i}—Mg1—O5	89.91 (8)	C9—C10—H10	119.9
O2—Mg1—O5	90.09 (8)	C10—C11—C12	120.4 (3)
O5^{i}—Mg1—O5	180.0	C10—C11—H11	119.8
O2^{i}—Mg1—O6^{i}	90.80 (7)	C12—C11—H11	119.8
O2—Mg1—O6^{i}	89.20 (7)	C7—C12—C11	118.9 (3)
O5^{i}—Mg1—O6^{i}	89.46 (8)	C7—C12—H12	120.5
O5—Mg1—O6^{i}	90.54 (8)	C11—C12—H12	120.5
O2^{i}—Mg1—O6	89.20 (7)	O5—C14—N4	123.7 (3)
O2—Mg1—O6	90.80 (7)	O5—C14—H14	118.1
O5^{i}—Mg1—O6	90.54 (8)	N4—C14—H14	118.1
O5—Mg1—O6	89.46 (8)	N4—C15—H15A	109.5
O6^{i}—Mg1—O6	180.0	N4—C15—H15B	109.5
O1^{ii}—Mg2—O1	180.0	H15A—C15—H15B	109.5
O1^{ii}—Mg2—O8	89.95 (8)	N4—C15—H15C	109.5
O1—Mg2—O8	90.05 (8)	H15A—C15—H15C	109.5
O1^{ii}—Mg2—O8^{ii}	90.05 (8)	H15B—C15—H15C	109.5
O1—Mg2—O8^{ii}	89.95 (8)	N4—C16—H16A	109.5
O8—Mg2—O8^{ii}	180.0	N4—C16—H16B	109.5
O1^{ii}—Mg2—O7	90.96 (7)	H16A—C16—H16B	109.5
O1—Mg2—O7	89.04 (7)	N4—C16—H16C	109.5
O8—Mg2—O7	89.98 (8)	H16A—C16—H16C	109.5
O8^{ii}—Mg2—O7	90.02 (8)	H16B—C16—H16C	109.5
O1^{ii}—Mg2—O7^{ii}	89.04 (7)	O6—C17—N2	124.8 (3)
O1—Mg2—O7^{ii}	90.96 (7)	O6—C17—H17	117.6
O8—Mg2—O7^{ii}	90.02 (8)	N2—C17—H17	117.6
O8^{ii}—Mg2—O7^{ii}	89.98 (8)	N2—C18—H18A	109.5
O7—Mg2—O7^{ii}	180.0	N2—C18—H18B	109.5
O2—P1—O1	120.34 (11)	H18A—C18—H18B	109.5
O2—P1—O4	105.57 (11)	N2—C18—H18C	109.5
O1—P1—O4	110.10 (11)	H18A—C18—H18C	109.5
O2—P1—O3	109.87 (10)	H18B—C18—H18C	109.5
O1—P1—O3	105.68 (11)	N2—C19—H19A	109.5
O4—P1—O3	104.22 (11)	N2—C19—H19B	109.5
C20—N1—C22	120.8 (3)	H19A—C19—H19B	109.5
C20—N1—C21	121.4 (3)	N2—C19—H19C	109.5
C22—N1—C21	117.6 (3)	H19A—C19—H19C	109.5
C17—N2—C18	121.7 (3)	H19B—C19—H19C	109.5
C17—N2—C19	121.6 (3)	O8—C20—N1	124.3 (3)

C18—N2—C19	116.4 (3)	O8—C20—H20	117.9
C23—N3—C24	121.5 (3)	N1—C20—H20	117.9
C23—N3—C25	121.3 (3)	N1—C21—H21A	109.5
C24—N3—C25	117.1 (2)	N1—C21—H21B	109.5
C14—N4—C15	120.9 (2)	H21A—C21—H21B	109.5
C14—N4—C16	121.9 (3)	N1—C21—H21C	109.5
C15—N4—C16	117.2 (2)	H21A—C21—H21C	109.5
P1—O1—Mg2	136.79 (11)	H21B—C21—H21C	109.5
P1—O2—Mg1	136.67 (11)	N1—C22—H22A	109.5
C7—O3—P1	125.70 (17)	N1—C22—H22B	109.5
C1—O4—P1	126.81 (18)	H22A—C22—H22B	109.5
C14—O5—Mg1	130.04 (19)	N1—C22—H22C	109.5
C17—O6—Mg1	127.64 (19)	H22A—C22—H22C	109.5
C23—O7—Mg2	126.37 (18)	H22B—C22—H22C	109.5
C20—O8—Mg2	130.27 (19)	O7—C23—N3	125.1 (3)
C6—C1—C2	121.5 (3)	O7—C23—H23	117.5
C6—C1—O4	123.0 (3)	N3—C23—H23	117.5
C2—C1—O4	115.4 (3)	N3—C24—H24A	109.5
C1—C2—C3	119.5 (3)	N3—C24—H24B	109.5
C1—C2—H2	120.2	H24A—C24—H24B	109.5
C3—C2—H2	120.2	N3—C24—H24C	109.5
C4—C3—C2	119.7 (3)	H24A—C24—H24C	109.5
C4—C3—H3	120.1	H24B—C24—H24C	109.5
C2—C3—H3	120.1	N3—C25—H25A	109.5
C3—C4—C5	120.3 (3)	N3—C25—H25B	109.5
C3—C4—H4	119.8	H25A—C25—H25B	109.5
C5—C4—H4	119.8	N3—C25—H25C	109.5
C4—C5—C6	120.6 (3)	H25A—C25—H25C	109.5
C4—C5—H5	119.7	H25B—C25—H25C	109.5
C6—C5—H5	119.7	F1—C1S—F3	107.7 (3)
C1—C6—C5	118.3 (3)	F1—C1S—F2	107.7 (3)
C1—C6—H6	120.8	F3—C1S—F2	108.0 (3)
C5—C6—H6	120.8	F1—C1S—S1	111.5 (3)
C8—C7—C12	121.2 (3)	F3—C1S—S1	111.4 (2)
C8—C7—O3	116.5 (3)	F2—C1S—S1	110.5 (3)
C12—C7—O3	122.3 (3)	O1S—S1—O2S	115.91 (17)
C7—C8—C9	119.7 (3)	O1S—S1—O3S	114.64 (16)
C7—C8—H8	120.1	O2S—S1—O3S	115.09 (16)
C9—C8—H8	120.1	O1S—S1—C1S	102.96 (17)
C10—C9—C8	119.6 (3)	O2S—S1—C1S	102.92 (16)
C10—C9—H9	120.2	O3S—S1—C1S	102.62 (18)

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