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μ-1,4-Diazabicyclo[2.2.2]octane-κ^2N:N'-bis[bis(*O*,*O*′-dicyclohexyl dithiophosphato-κ^2S,S')cadmium(II)]

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.018 Å
Disorder in main residue
R factor = 0.065
wR factor = 0.244
Data-to-parameter ratio = 14.5

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

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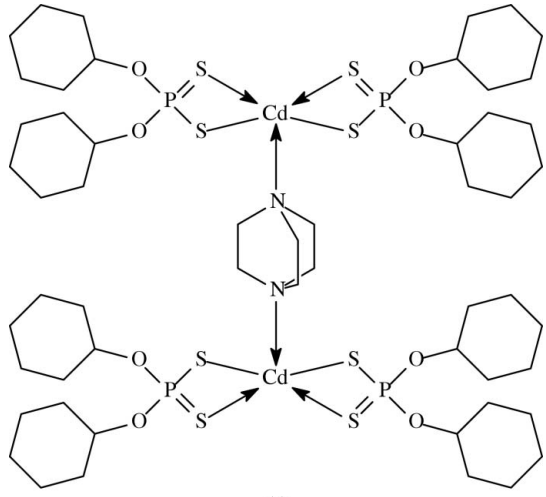
The dinuclear title molecule, $[Cd_2(C_{12}H_{22}O_2PS_2)_4(C_6H_{12}N_2)]$, is disordered and located on a centre of inversion, and features a coordination geometry intermediate between square-pyramidal and trigonal-bipyramidal.

Comment

Structures closely related to the title complex, (I), *viz.* $\{M_2[(i\text{-}C_3H_7O)_2PS_2]_4(C_6H_{12}N_2)\}$ for *M* = Zn (Ellis *et al.*, 2007) and Cd (Ellis & Tiekink, 2006), have been reported recently in connection with ongoing studies aimed at determining the principles of supramolecular aggregation for the zinc-triad dithiophosphates ($S_2P(OR)_2$), and their adducts (Lai, Liu & Tiekink, 2004; Lai & Tiekink, 2004, 2006; Tiekink, 2003).



(I)

The structure of (I) (Fig. 1) is similar to that of the aforementioned structures, $\{M_2[(i\text{-}C_3H_7O)_2PS_2]_4(C_6H_{12}N_2)\}$, in particular the Cd analogue. The complex is located on a centre of inversion and features two $Cd[S_2P(OCy)_2]_2$ units bridged by a disordered 1,4-diazabicyclo[2.2.2]octane (dabco) ligand. A heavily distorted coordination geometry is found for Cd as both dithiophosphate ligands form asymmetric Cd—S bonds (Table 1). The $CdNS_4$ coordination geometry is intermediate between square-pyramidal (SP) and trigonal-pyramidal (TP), as seen in the value of τ = 0.51; τ = 0.0 and 1.0 for ideal SP and TP, respectively (Addison *et al.*, 1984).

Experimental

Compound (I) was prepared by refluxing the parent $Cd[S_2P(OCy)_2]_2$ compound with 1,4-diazabicyclo[2.2.2]octane (Aldrich) according to a literature procedure (Lai & Tiekink, 2004). Colourless crystals were

isolated by the slow evaporation of a $CHCl_3$/ethanol (3:1) solution of the compound (m.p. 468–470 K). IR (KBr disc): ν(C—O) 1152 (*w*), ν(P—O) 958 (*s*), ν(P—S)$_{asym}$ 657 (*s*), ν(P—S)$_{sym}$ 577 (*s*) cm^{-1}.

Crystal data

$[Cd_2(C_{12}H_{22}O_2PS_2)_4(C_6H_{12}N_2)]$
M_r = 1510.52
Monoclinic, $C2/c$
a = 23.1399 (12) Å
b = 20.5858 (12) Å
c = 16.0730 (6) Å
β = 116.951 (3)°
V = 6824.9 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 123 (2) K
0.50 × 0.10 × 0.07 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.730, T_{max} = 1
(expected range = 0.680–0.932)
30800 measured reflections
6023 independent reflections
3618 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.244
S = 1.08
6023 reflections
416 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −1.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.318 (7)	Cd1—S3	2.521 (2)
Cd1—S1	2.530 (3)	Cd1—S4	2.818 (3)
Cd1—S2	2.760 (3)		
N1—Cd1—S1	110.83 (16)	S1—Cd1—S3	136.60 (10)
N1—Cd1—S2	94.81 (19)	S1—Cd1—S4	99.91 (9)
N1—Cd1—S3	112.54 (16)	S2—Cd1—S3	96.87 (9)
N1—Cd1—S4	97.53 (19)	S2—Cd1—S4	167.41 (9)
S1—Cd1—S2	77.89 (9)	S3—Cd1—S4	76.08 (8)

For the cyclohexyl rings, the 1,2 C—C distances were restrained to 1.54 (1)Å and the 1,3-related distances to 2.51 (1)Å. One of them was refined as disordered over two positions with an occupancy factor for the major component of 0.62 (1). The C atoms of the dabco ligand, which lies about an inversion centre, are disordered; the occupancy was constrained by symmetry to be 0.5. The N—C distances were restrained to 1.45 (1)Å and the C—C distances to 1.50 (1)Å. The C-bound H atoms were included in the riding-model approximation, with C—H = 0.99–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C). The final difference Fourier map had a large residual electron-density peak **near** C5 atom and a deep hole **near** Cd1. The largest peak in the final difference map was 0.4 Å from C5 and the deepest hole was 1.0 Å from Cd1.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *PATTY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

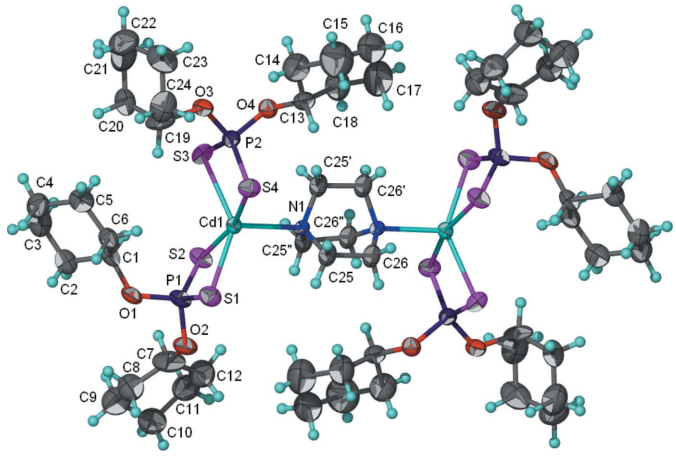


Figure 1
The molecular structure of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The minor disorder componenent of the cyclohexyl ring is not shown, and neither is one disorder component of dabco. Unlabelled atoms are generated by the symmetry operator (1 − x, 1 − y, 1 − z).

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supporting information

Acta Cryst. (2007). E**63**, m806–m807 [https://doi.org/10.1107/S1600536807007155]

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Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 23.1399$ (12) Å
$b = 20.5858$ (12) Å
$c = 16.0730$ (6) Å
$\beta = 116.951$ (3)°
$V = 6824.9$ (6) Å^3
$Z = 4$
$F(000) = 3144$
$D_x = 1.470$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 7655 reflections
$\theta = 1.0$–$27.5°$
$\mu = 1.01$ mm^{-1}
$T = 123$ K
Needle, colourless
0.50 × 0.10 × 0.07 mm

Data collection

Bruker–Nonius 95mm CCD camera on κ-goniostat diffractometer
Radiation source: Bruker-Nonius FR591 rotating-anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.730$, $T_{max} = 1$
30800 measured reflections
6023 independent reflections
3618 reflections with $I > 2\sigma(I)$
$R_{int} = 0.095$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
$h = -27\rightarrow27$
$k = -24\rightarrow23$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.244$
$S = 1.08$
6023 reflections
416 parameters
273 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
$w = 1/[\sigma^2(F_o^2) + (0.1455P)^2 + 7.331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.21$ e Å^{-3}
$\Delta\rho_{min} = -1.25$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.40925 (4)	0.62514 (3)	0.54530 (5)	0.0449 (3)	
S1	0.36134 (14)	0.70473 (14)	0.41105 (18)	0.0585 (7)	
S2	0.50553 (12)	0.71778 (13)	0.59674 (19)	0.0540 (7)	
S3	0.41221 (12)	0.61255 (13)	0.70318 (16)	0.0501 (7)	
S4	0.29845 (13)	0.55013 (13)	0.50894 (16)	0.0517 (7)	
P1	0.43363 (13)	0.76372 (13)	0.49274 (19)	0.0508 (7)	
P2	0.34330 (11)	0.54571 (12)	0.64647 (16)	0.0402 (6)	
O1	0.4079 (3)	0.8226 (3)	0.5296 (5)	0.0550 (18)	
O2	0.4545 (4)	0.7992 (4)	0.4223 (5)	0.065 (2)	
O3	0.2951 (3)	0.5494 (3)	0.6929 (4)	0.0508 (17)	
O4	0.3760 (3)	0.4776 (3)	0.6854 (4)	0.0499 (17)	
N1	0.4680 (4)	0.5451 (3)	0.5156 (4)	0.0421 (19)	
C1	0.3999 (4)	0.8193 (4)	0.6133 (6)	0.050 (2)	
H1	0.4343	0.7908	0.6601	0.060*	
C2	0.4054 (5)	0.8865 (4)	0.6535 (7)	0.065 (3)	
H2A	0.4476	0.9053	0.6642	0.078*	
H2B	0.3709	0.9141	0.6066	0.078*	
C3	0.4002 (5)	0.8900 (6)	0.7426 (7)	0.077 (4)	
H3A	0.4059	0.9354	0.7652	0.093*	
H3B	0.4344	0.8631	0.7909	0.093*	
C4	0.3328 (5)	0.8649 (5)	0.7242 (8)	0.072 (3)	
H4A	0.3288	0.8629	0.7829	0.087*	
H4B	0.2982	0.8935	0.6794	0.087*	
C5	0.3284 (5)	0.7993 (5)	0.6846 (7)	0.070 (3)	
H5A	0.2869	0.7798	0.6757	0.084*	
H5B	0.3637	0.7726	0.7317	0.084*	
C6	0.3323 (4)	0.7930 (4)	0.5939 (6)	0.053 (3)	
H6A	0.2976	0.8188	0.5444	0.064*	
H6B	0.3276	0.7470	0.5739	0.064*	
C7	0.5046 (5)	0.8451 (5)	0.4505 (9)	0.092 (4)	
H7A	0.5224	0.8431	0.5199	0.110*	0.623 (14)
H7B	0.4877	0.8829	0.4719	0.110*	0.377 (14)
C8	0.4890 (6)	0.9157 (6)	0.4329 (15)	0.087 (7)	0.623 (14)
H8A	0.4613	0.9285	0.4625	0.104*	0.623 (14)
H8B	0.4636	0.9227	0.3649	0.104*	0.623 (14)
C9	0.5485 (8)	0.9597 (6)	0.4699 (14)	0.096 (8)	0.623 (14)
H9A	0.5702	0.9588	0.5390	0.115*	0.623 (14)
H9B	0.5351	1.0049	0.4495	0.115*	0.623 (14)
C8′	0.4968 (10)	0.8667 (11)	0.3531 (9)	0.079 (10)	0.377 (14)
H8′1	0.5204	0.8364	0.3314	0.095*	0.377 (14)
H8′2	0.4504	0.8663	0.3070	0.095*	0.377 (14)
C9′	0.5245 (9)	0.9359 (10)	0.3620 (13)	0.101 (13)	0.377 (14)
H9′1	0.5201	0.9505	0.3007	0.121*	0.377 (14)
H9′2	0.4999	0.9663	0.3818	0.121*	0.377 (14)
C10	0.5958 (6)	0.9365 (5)	0.4335 (9)	0.095 (4)	

H10A	0.6331	0.9665	0.4539	0.114*	0.623 (14)
H10B	0.5738	0.9350	0.3644	0.114*	0.623 (14)
H10C	0.6134	0.9810	0.4390	0.114*	0.377 (14)
H10D	0.6206	0.9074	0.4125	0.114*	0.377 (14)
C11	0.6191 (6)	0.8676 (7)	0.4741 (14)	0.093 (7)	0.623 (14)
H11A	0.6517	0.8517	0.4550	0.111*	0.623 (14)
H11B	0.6396	0.8692	0.5431	0.111*	0.623 (14)
C12	0.5613 (7)	0.8215 (5)	0.4380 (15)	0.089 (7)	0.623 (14)
H12A	0.5469	0.8137	0.3708	0.107*	0.623 (14)
H12B	0.5756	0.7794	0.4706	0.107*	0.623 (14)
C11′	0.6033 (10)	0.9138 (12)	0.5291 (9)	0.087 (11)	0.377 (14)
H11C	0.5788	0.9429	0.5506	0.105*	0.377 (14)
H11D	0.6496	0.9150	0.5756	0.105*	0.377 (14)
C12′	0.5770 (9)	0.8435 (11)	0.5191 (15)	0.133 (18)	0.377 (14)
H12C	0.6004	0.8145	0.4953	0.159*	0.377 (14)
H12D	0.5834	0.8269	0.5805	0.159*	0.377 (14)
C13	0.3492 (5)	0.4155 (4)	0.6406 (7)	0.065 (3)	
H13	0.3305	0.4197	0.5713	0.078*	
C14	0.2985 (6)	0.3892 (5)	0.6677 (10)	0.097 (5)	
H14A	0.2613	0.4196	0.6468	0.117*	
H14B	0.3175	0.3850	0.7364	0.117*	
C15	0.2749 (6)	0.3221 (6)	0.6215 (13)	0.146 (7)	
H15A	0.2436	0.3038	0.6414	0.175*	
H15B	0.2525	0.3272	0.5528	0.175*	
C16	0.3309 (8)	0.2761 (5)	0.6481 (11)	0.125 (6)	
H16A	0.3150	0.2353	0.6122	0.150*	
H16B	0.3483	0.2653	0.7151	0.150*	
C17	0.3854 (7)	0.3031 (6)	0.6304 (12)	0.151 (7)	
H17A	0.3701	0.3080	0.5624	0.181*	
H17B	0.4222	0.2722	0.6544	0.181*	
C18	0.4085 (5)	0.3693 (6)	0.6783 (11)	0.110 (5)	
H18A	0.4428	0.3870	0.6642	0.132*	
H18B	0.4263	0.3646	0.7468	0.132*	
C19	0.2541 (5)	0.6112 (6)	0.6816 (6)	0.074 (4)	
H19	0.2528	0.6389	0.6297	0.089*	
C20	0.2806 (5)	0.6495 (5)	0.7721 (7)	0.074 (3)	
H20A	0.3264	0.6606	0.7909	0.088*	
H20B	0.2561	0.6906	0.7613	0.088*	
C21	0.2767 (7)	0.6133 (7)	0.8507 (7)	0.123 (6)	
H21A	0.2891	0.6426	0.9050	0.148*	
H21B	0.3074	0.5764	0.8700	0.148*	
C22	0.2082 (6)	0.5882 (7)	0.8201 (8)	0.108 (5)	
H22A	0.2065	0.5639	0.8722	0.130*	
H22B	0.1780	0.6254	0.8046	0.130*	
C23	0.1868 (6)	0.5439 (6)	0.7356 (9)	0.103 (5)	
H23A	0.1422	0.5283	0.7170	0.123*	
H23B	0.2158	0.5057	0.7516	0.123*	
C24	0.1889 (5)	0.5806 (7)	0.6545 (7)	0.101 (5)	

H24A	0.1788	0.5502	0.6020	0.121*	
H24B	0.1552	0.6149	0.6328	0.121*	
C25	0.4381 (9)	0.5250 (10)	0.4200 (8)	0.051 (5)	0.50
H25A	0.4342	0.5629	0.3799	0.061*	0.50
H25B	0.3938	0.5089	0.4030	0.061*	0.50
C26	0.4757 (9)	0.4725 (11)	0.4014 (10)	0.065 (6)	0.50
H26A	0.4478	0.4338	0.3759	0.078*	0.50
H26B	0.4889	0.4878	0.3540	0.078*	0.50
C25′	0.4839 (9)	0.4923 (7)	0.5832 (10)	0.039 (4)	0.50
H25C	0.4435	0.4748	0.5812	0.046*	0.50
H25D	0.5109	0.5094	0.6467	0.046*	0.50
C26′	0.5200 (12)	0.4381 (9)	0.5633 (13)	0.062 (6)	0.50
H26C	0.5618	0.4303	0.6192	0.075*	0.50
H26D	0.4941	0.3977	0.5493	0.075*	0.50
C25"	0.5354 (6)	0.5683 (8)	0.5416 (14)	0.054 (5)	0.50
H25E	0.5563	0.5836	0.6071	0.065*	0.50
H25F	0.5341	0.6049	0.5008	0.065*	0.50
C26"	0.5736 (8)	0.5120 (8)	0.5299 (19)	0.081 (7)	0.50
H26E	0.5949	0.5265	0.4918	0.098*	0.50
H26F	0.6079	0.4991	0.5920	0.098*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0605 (5)	0.0340 (4)	0.0584 (5)	0.0081 (3)	0.0430 (4)	0.0054 (3)
S1	0.0575 (18)	0.0574 (18)	0.0528 (15)	0.0076 (14)	0.0183 (13)	0.0105 (13)
S2	0.0385 (15)	0.0495 (17)	0.0689 (16)	0.0023 (12)	0.0198 (13)	0.0152 (13)
S3	0.0448 (15)	0.0660 (18)	0.0421 (13)	−0.0084 (13)	0.0219 (11)	−0.0092 (12)
S4	0.0511 (16)	0.0559 (17)	0.0382 (12)	−0.0092 (13)	0.0117 (11)	0.0003 (11)
P1	0.0487 (17)	0.0437 (16)	0.0618 (16)	0.0046 (13)	0.0267 (14)	0.0185 (13)
P2	0.0378 (14)	0.0440 (15)	0.0447 (13)	0.0046 (11)	0.0238 (11)	0.0055 (11)
O1	0.067 (5)	0.038 (4)	0.068 (4)	0.003 (3)	0.037 (4)	0.017 (3)
O2	0.078 (5)	0.057 (5)	0.068 (5)	0.001 (4)	0.041 (4)	0.019 (4)
O3	0.049 (4)	0.055 (4)	0.061 (4)	0.017 (3)	0.036 (3)	0.021 (3)
O4	0.052 (4)	0.049 (4)	0.055 (4)	0.009 (3)	0.029 (3)	0.007 (3)
N1	0.063 (5)	0.034 (4)	0.050 (4)	0.008 (4)	0.043 (4)	0.006 (3)
C1	0.046 (5)	0.034 (5)	0.066 (6)	0.000 (4)	0.022 (4)	0.006 (4)
C2	0.055 (6)	0.055 (6)	0.074 (6)	−0.002 (5)	0.020 (5)	−0.001 (5)
C3	0.073 (7)	0.075 (7)	0.082 (7)	0.005 (6)	0.034 (6)	−0.012 (6)
C4	0.068 (7)	0.076 (7)	0.078 (6)	0.013 (6)	0.038 (5)	0.000 (5)
C5	0.052 (6)	0.076 (7)	0.090 (7)	0.005 (5)	0.039 (5)	0.014 (6)
C6	0.049 (6)	0.045 (6)	0.071 (6)	0.005 (4)	0.031 (5)	0.006 (5)
C7	0.078 (7)	0.109 (9)	0.103 (8)	−0.015 (7)	0.055 (6)	0.028 (7)
C8	0.077 (10)	0.087 (11)	0.102 (11)	0.000 (8)	0.047 (8)	0.003 (8)
C9	0.082 (11)	0.106 (12)	0.104 (11)	−0.018 (9)	0.046 (8)	−0.005 (9)
C8′	0.078 (13)	0.091 (14)	0.077 (13)	−0.018 (9)	0.042 (10)	0.019 (9)
C9′	0.111 (16)	0.102 (16)	0.094 (15)	0.013 (10)	0.049 (11)	0.002 (10)
C10	0.103 (9)	0.087 (8)	0.110 (8)	−0.011 (7)	0.061 (7)	0.002 (7)

C11	0.093 (11)	0.101 (12)	0.096 (11)	−0.006 (8)	0.053 (8)	0.004 (8)
C12	0.083 (10)	0.088 (11)	0.100 (11)	0.002 (8)	0.046 (8)	0.000 (8)
C11′	0.094 (15)	0.083 (15)	0.091 (14)	−0.012 (10)	0.047 (10)	−0.001 (10)
C12′	0.13 (2)	0.13 (2)	0.13 (2)	−0.014 (11)	0.061 (12)	0.011 (11)
C13	0.096 (8)	0.055 (6)	0.051 (5)	−0.005 (6)	0.039 (5)	0.001 (5)
C14	0.106 (9)	0.089 (8)	0.115 (8)	−0.027 (7)	0.065 (7)	−0.017 (7)
C15	0.141 (11)	0.133 (11)	0.159 (11)	−0.027 (9)	0.064 (8)	−0.020 (9)
C16	0.167 (11)	0.098 (9)	0.111 (9)	−0.001 (8)	0.063 (8)	−0.009 (7)
C17	0.187 (12)	0.124 (11)	0.142 (10)	0.017 (9)	0.077 (9)	−0.018 (8)
C18	0.124 (10)	0.096 (9)	0.113 (9)	0.019 (7)	0.057 (7)	−0.006 (7)
C19	0.060 (6)	0.113 (8)	0.070 (6)	0.019 (6)	0.049 (5)	0.040 (6)
C20	0.070 (7)	0.058 (6)	0.095 (7)	0.005 (5)	0.040 (6)	−0.006 (6)
C21	0.143 (10)	0.125 (10)	0.114 (9)	0.031 (8)	0.069 (8)	−0.011 (7)
C22	0.111 (9)	0.133 (10)	0.107 (8)	0.028 (8)	0.071 (7)	0.025 (7)
C23	0.082 (8)	0.088 (8)	0.159 (10)	−0.008 (6)	0.073 (7)	0.024 (7)
C24	0.084 (8)	0.119 (9)	0.088 (7)	0.011 (7)	0.029 (6)	−0.015 (7)
C25	0.056 (9)	0.050 (9)	0.035 (7)	0.014 (8)	0.011 (7)	−0.008 (7)
C26	0.075 (10)	0.063 (10)	0.043 (8)	0.008 (9)	0.015 (7)	−0.004 (8)
C25′	0.039 (8)	0.041 (8)	0.039 (7)	0.022 (7)	0.020 (6)	−0.001 (6)
C26′	0.072 (10)	0.070 (10)	0.060 (9)	0.018 (8)	0.043 (8)	0.006 (8)
C25"	0.052 (9)	0.054 (9)	0.059 (9)	0.010 (7)	0.028 (7)	−0.014 (7)
C26"	0.071 (11)	0.085 (12)	0.097 (11)	0.003 (9)	0.047 (9)	−0.020 (9)

Geometric parameters (Å, º)

Cd1—N1	2.318 (7)	C10—H10D	0.9900
Cd1—S1	2.530 (3)	C11—C12	1.524 (10)
Cd1—S2	2.760 (3)	C11—H11A	0.9900
Cd1—S3	2.521 (2)	C11—H11B	0.9900
Cd1—S4	2.818 (3)	C12—H12A	0.9900
S1—P1	2.002 (4)	C12—H12B	0.9900
S2—P1	1.984 (4)	C11′—C12′	1.549 (11)
S3—P2	1.987 (4)	C11′—H11C	0.9900
S4—P2	1.973 (3)	C11′—H11D	0.9900
P1—O1	1.580 (8)	C12′—H12C	0.9900
P1—O2	1.594 (7)	C12′—H12D	0.9900
P2—O4	1.581 (7)	C13—C14	1.525 (9)
P2—O3	1.601 (6)	C13—C18	1.549 (9)
O1—C1	1.441 (10)	C13—H13	1.0000
O2—C7	1.404 (12)	C14—C15	1.547 (9)
O3—C19	1.548 (13)	C14—H14A	0.9900
O4—C13	1.460 (11)	C14—H14B	0.9900
N1—C26^{i}	1.426 (10)	C15—C16	1.502 (9)
N1—C25	1.431 (10)	C15—H15A	0.9900
N1—C26′^{i}	1.459 (10)	C15—H15B	0.9900
N1—C25′	1.462 (10)	C16—C17	1.518 (10)
N1—C26"^{i}	1.485 (10)	C16—H16A	0.9900
N1—C25"	1.499 (10)	C16—H16B	0.9900

C1—C2	1.508 (8)	C17—C18	1.538 (9)
C1—C6	1.548 (8)	C17—H17A	0.9900
C1—H1	1.0000	C17—H17B	0.9900
C2—C3	1.492 (8)	C18—H18A	0.9900
C2—H2A	0.9900	C18—H18B	0.9900
C2—H2B	0.9900	C19—C24	1.506 (9)
C3—C4	1.539 (9)	C19—C20	1.518 (9)
C3—H3A	0.9900	C19—H19	1.0000
C3—H3B	0.9900	C20—C21	1.502 (9)
C4—C5	1.478 (9)	C20—H20A	0.9900
C4—H4A	0.9900	C20—H20B	0.9900
C4—H4B	0.9900	C21—C22	1.522 (9)
C5—C6	1.504 (8)	C21—H21A	0.9900
C5—H5A	0.9900	C21—H21B	0.9900
C5—H5B	0.9900	C22—C23	1.520 (9)
C6—H6A	0.9900	C22—H22A	0.9900
C6—H6B	0.9900	C22—H22B	0.9900
C7—C8	1.493 (9)	C23—C24	1.526 (9)
C7—C12	1.493 (9)	C23—H23A	0.9900
C7—C12′	1.533 (11)	C23—H23B	0.9900
C7—C8′	1.556 (10)	C24—H24A	0.9900
C7—H7A	1.0000	C24—H24B	0.9900
C7—H7B	1.0000	C25—C26	1.500 (10)
C8—C9	1.526 (10)	C25—H25A	0.9900
C8—H8A	0.9900	C25—H25B	0.9900
C8—H8B	0.9900	C26—N1^{i}	1.426 (10)
C9—C10	1.532 (10)	C26—H26A	0.9900
C9—H9A	0.9900	C26—H26B	0.9900
C9—H9B	0.9900	C25′—C26′	1.511 (10)
C8′—C9′	1.543 (10)	C25′—H25C	0.9900
C8′—H8′1	0.9900	C25′—H25D	0.9900
C8′—H8′2	0.9900	C26′—N1^{i}	1.459 (10)
C9′—C10	1.523 (10)	C26′—H26C	0.9900
C9′—H9′1	0.9900	C26′—H26D	0.9900
C9′—H9′2	0.9900	C25"—C26"	1.519 (10)
C10—C11′	1.539 (10)	C25"—H25E	0.9900
C10—C11	1.553 (10)	C25"—H25F	0.9900
C10—H10A	0.9900	C26"—N1^{i}	1.485 (10)
C10—H10B	0.9900	C26"—H26E	0.9900
C10—H10C	0.9900	C26"—H26F	0.9900

N1—Cd1—S1	110.83 (16)	H10A—C10—H10B	108.5
N1—Cd1—S2	94.81 (19)	C9′—C10—H10C	109.6
N1—Cd1—S3	112.54 (16)	C9—C10—H10C	90.8
N1—Cd1—S4	97.53 (19)	C11′—C10—H10C	109.6
S1—Cd1—S2	77.89 (9)	C11—C10—H10C	139.2
S1—Cd1—S3	136.60 (10)	H10B—C10—H10C	96.4
S1—Cd1—S4	99.91 (9)	C9′—C10—H10D	109.6

S2—Cd1—S3	96.87 (9)	C9—C10—H10D	160.8
S2—Cd1—S4	167.41 (9)	C11′—C10—H10D	109.6
S3—Cd1—S4	76.08 (8)	C11—C10—H10D	56.3
P1—S1—Cd1	85.45 (12)	H10A—C10—H10D	86.3
P1—S2—Cd1	79.76 (12)	H10B—C10—H10D	71.4
P2—S3—Cd1	87.67 (11)	H10C—C10—H10D	108.1
P2—S4—Cd1	79.96 (11)	C12—C11—C10	109.3 (8)
O1—P1—O2	101.7 (4)	C12—C11—H11A	109.8
O1—P1—S2	111.4 (3)	C10—C11—H11A	109.8
O2—P1—S2	114.1 (3)	C12—C11—H11B	109.8
O1—P1—S1	111.5 (3)	C10—C11—H11B	109.8
O2—P1—S1	104.1 (3)	H11A—C11—H11B	108.3
S2—P1—S1	113.32 (17)	C7—C12—C11	114.8 (8)
O4—P2—O3	99.6 (3)	C7—C12—H12A	108.6
O4—P2—S4	113.5 (3)	C11—C12—H12A	108.6
O3—P2—S4	113.3 (3)	C7—C12—H12B	108.6
O4—P2—S3	107.0 (3)	C11—C12—H12B	108.6
O3—P2—S3	109.7 (3)	H12A—C12—H12B	107.5
S4—P2—S3	112.79 (15)	C10—C11′—C12′	108.6 (9)
C1—O1—P1	123.0 (6)	C10—C11′—H11C	110.0
C7—O2—P1	123.5 (7)	C12′—C11′—H11C	110.0
C19—O3—P2	120.3 (5)	C10—C11′—H11D	110.0
C13—O4—P2	124.1 (6)	C12′—C11′—H11D	110.0
C26^{i}—N1—C25	136.3 (7)	H11C—C11′—H11D	108.3
C26^{i}—N1—C26′^{i}	114.9 (14)	C7—C12′—C11′	107.7 (10)
C25—N1—C26′^{i}	47.5 (13)	C7—C12′—H12C	110.2
C26^{i}—N1—C25′	45.5 (12)	C11′—C12′—H12C	110.2
C25—N1—C25′	114.7 (12)	C7—C12′—H12D	110.2
C26′^{i}—N1—C25′	137.7 (7)	C11′—C12′—H12D	110.2
C26^{i}—N1—C26"^{i}	111.8 (15)	H12C—C12′—H12D	108.5
C25—N1—C26"^{i}	49.6 (13)	O4—C13—C14	112.3 (8)
C26′^{i}—N1—C26"^{i}	95.5 (15)	O4—C13—C18	104.0 (8)
C25′—N1—C26"^{i}	70.4 (14)	C14—C13—C18	109.3 (7)
C26^{i}—N1—C25"	55.0 (13)	O4—C13—H13	110.4
C25—N1—C25"	109.0 (13)	C14—C13—H13	110.4
C26′^{i}—N1—C25"	65.2 (13)	C18—C13—H13	110.4
C25′—N1—C25"	98.6 (12)	C13—C14—C15	109.2 (7)
C26"^{i}—N1—C25"	138.5 (8)	C13—C14—H14A	109.8
C26^{i}—N1—Cd1	111.1 (8)	C15—C14—H14A	109.8
C25—N1—Cd1	112.6 (8)	C13—C14—H14B	109.8
C26′^{i}—N1—Cd1	111.8 (7)	C15—C14—H14B	109.8
C25′—N1—Cd1	110.5 (6)	H14A—C14—H14B	108.3
C26"^{i}—N1—Cd1	110.8 (8)	C16—C15—C14	110.9 (8)
C25"—N1—Cd1	110.5 (7)	C16—C15—H15A	109.5
O1—C1—C2	109.6 (7)	C14—C15—H15A	109.5
O1—C1—C6	112.0 (7)	C16—C15—H15B	109.5
C2—C1—C6	106.8 (6)	C14—C15—H15B	109.5
O1—C1—H1	109.5	H15A—C15—H15B	108.1

C2—C1—H1	109.5	C15—C16—C17	113.5 (8)
C6—C1—H1	109.5	C15—C16—H16A	108.9
C3—C2—C1	115.3 (7)	C17—C16—H16A	108.9
C3—C2—H2A	108.4	C15—C16—H16B	108.9
C1—C2—H2A	108.4	C17—C16—H16B	108.9
C3—C2—H2B	108.4	H16A—C16—H16B	107.7
C1—C2—H2B	108.4	C16—C17—C18	111.2 (8)
H2A—C2—H2B	107.5	C16—C17—H17A	109.4
C2—C3—C4	108.3 (7)	C18—C17—H17A	109.4
C2—C3—H3A	110.0	C16—C17—H17B	109.4
C4—C3—H3A	110.0	C18—C17—H17B	109.4
C2—C3—H3B	110.0	H17A—C17—H17B	108.0
C4—C3—H3B	110.0	C17—C18—C13	107.7 (8)
H3A—C3—H3B	108.4	C17—C18—H18A	110.2
C5—C4—C3	104.8 (7)	C13—C18—H18A	110.2
C5—C4—H4A	110.8	C17—C18—H18B	110.2
C3—C4—H4A	110.8	C13—C18—H18B	110.2
C5—C4—H4B	110.8	H18A—C18—H18B	108.5
C3—C4—H4B	110.8	C24—C19—C20	114.2 (7)
H4A—C4—H4B	108.9	C24—C19—O3	99.8 (9)
C4—C5—C6	118.2 (7)	C20—C19—O3	110.7 (8)
C4—C5—H5A	107.8	C24—C19—H19	110.5
C6—C5—H5A	107.8	C20—C19—H19	110.5
C4—C5—H5B	107.8	O3—C19—H19	110.5
C6—C5—H5B	107.8	C21—C20—C19	113.4 (7)
H5A—C5—H5B	107.1	C21—C20—H20A	108.9
C5—C6—C1	105.8 (6)	C19—C20—H20A	108.9
C5—C6—H6A	110.6	C21—C20—H20B	108.9
C1—C6—H6A	110.6	C19—C20—H20B	108.9
C5—C6—H6B	110.6	H20A—C20—H20B	107.7
C1—C6—H6B	110.6	C20—C21—C22	110.3 (8)
H6A—C6—H6B	108.7	C20—C21—H21A	109.6
O2—C7—C8	120.1 (10)	C22—C21—H21A	109.6
O2—C7—C12	112.6 (10)	C20—C21—H21B	109.6
C8—C7—C12	116.3 (7)	C22—C21—H21B	109.6
O2—C7—C12′	133.7 (10)	H21A—C21—H21B	108.1
C8—C7—C12′	104.4 (10)	C23—C22—C21	111.2 (8)
C12—C7—C12′	49.5 (13)	C23—C22—H22A	109.4
O2—C7—C8′	99.5 (9)	C21—C22—H22A	109.4
C8—C7—C8′	68.0 (13)	C23—C22—H22B	109.4
C12—C7—C8′	70.6 (13)	C21—C22—H22B	109.4
C12′—C7—C8′	108.7 (9)	H22A—C22—H22B	108.0
O2—C7—H7A	101.1	C22—C23—C24	110.1 (7)
C8—C7—H7A	101.1	C22—C23—H23A	109.6
C12—C7—H7A	101.1	C24—C23—H23A	109.6
C12′—C7—H7A	55.5	C22—C23—H23B	109.6
C8′—C7—H7A	159.3	C24—C23—H23B	109.6
O2—C7—H7B	103.9	H23A—C23—H23B	108.2

C12—C7—H7B	143.5	C19—C24—C23	112.0 (7)
C12′—C7—H7B	103.9	C19—C24—H24A	109.2
C8′—C7—H7B	103.9	C23—C24—H24A	109.2
H7A—C7—H7B	71.0	C19—C24—H24B	109.2
C7—C8—C9	113.9 (8)	C23—C24—H24B	109.2
C7—C8—H8A	108.8	H24A—C24—H24B	107.9
C9—C8—H8A	108.8	N1—C25—C26	112.4 (12)
C7—C8—H8B	108.8	N1—C25—H25A	109.1
C9—C8—H8B	108.8	C26—C25—H25A	109.1
H8A—C8—H8B	107.7	N1—C25—H25B	109.1
C8—C9—C10	110.0 (8)	C26—C25—H25B	109.1
C8—C9—H9A	109.7	H25A—C25—H25B	107.8
C10—C9—H9A	109.7	N1^{i}—C26—C25	111.3 (12)
C8—C9—H9B	109.7	N1^{i}—C26—H26A	109.4
C10—C9—H9B	109.7	C25—C26—H26A	109.4
H9A—C9—H9B	108.2	N1^{i}—C26—H26B	109.4
C9′—C8′—C7	108.4 (9)	C25—C26—H26B	109.4
C9′—C8′—H8′1	110.0	H26A—C26—H26B	108.0
C7—C8′—H8′1	110.0	N1—C25′—C26′	111.7 (10)
C9′—C8′—H8′2	110.0	N1—C25′—H25C	109.3
C7—C8′—H8′2	110.0	C26′—C25′—H25C	109.3
H8′1—C8′—H8′2	108.4	N1—C25′—H25D	109.3
C10—C9′—C8′	109.9 (10)	C26′—C25′—H25D	109.3
C10—C9′—H9′1	109.7	H25C—C25′—H25D	107.9
C8′—C9′—H9′1	109.7	N1^{i}—C26′—C25′	110.5 (11)
C10—C9′—H9′2	109.7	N1^{i}—C26′—H26C	109.5
C8′—C9′—H9′2	109.7	C25′—C26′—H26C	109.5
H9′1—C9′—H9′2	108.2	N1^{i}—C26′—H26D	109.5
C9′—C10—C9	64.8 (13)	C25′—C26′—H26D	109.5
C9′—C10—C11′	110.2 (9)	H26C—C26′—H26D	108.1
C9—C10—C11′	59.4 (13)	N1—C25"—C26"	108.2 (12)
C9′—C10—C11	111.1 (9)	N1—C25"—H25E	110.0
C9—C10—C11	107.2 (8)	C26"—C25"—H25E	110.0
C11′—C10—C11	56.0 (13)	N1—C25"—H25F	110.0
C9′—C10—H10A	137.6	C26"—C25"—H25F	110.0
C9—C10—H10A	110.3	H25E—C25"—H25F	108.4
C11′—C10—H10A	99.9	N1^{i}—C26"—C25"	112.5 (13)
C11—C10—H10A	110.3	N1^{i}—C26"—H26E	109.1
C9′—C10—H10B	47.5	C25"—C26"—H26E	109.1
C9—C10—H10B	110.3	N1^{i}—C26"—H26F	109.1
C11′—C10—H10B	151.5	C25"—C26"—H26F	109.1
C11—C10—H10B	110.3	H26E—C26"—H26F	107.8

N1—Cd1—S1—P1	−102.5 (2)	P1—O2—C7—C12′	58 (2)
S3—Cd1—S1—P1	75.32 (17)	P1—O2—C7—C8′	−174.2 (12)
S2—Cd1—S1—P1	−11.87 (12)	O2—C7—C8—C9	178.4 (12)
S4—Cd1—S1—P1	155.50 (12)	C12—C7—C8—C9	−40.1 (19)
N1—Cd1—S2—P1	122.44 (19)	C12′—C7—C8—C9	11.5 (18)

S3—Cd1—S2—P1	−124.14 (13)	C8′—C7—C8—C9	−93.2 (14)
S1—Cd1—S2—P1	12.14 (12)	C7—C8—C9—C10	52.5 (18)
S4—Cd1—S2—P1	−69.0 (4)	O2—C7—C8′—C9′	155.1 (14)
N1—Cd1—S3—P2	−80.8 (2)	C8—C7—C8′—C9′	36.4 (13)
S1—Cd1—S3—P2	101.45 (16)	C12—C7—C8′—C9′	−94.1 (13)
S2—Cd1—S3—P2	−178.93 (11)	C12′—C7—C8′—C9′	−62.0 (17)
S4—Cd1—S3—P2	11.68 (11)	C7—C8′—C9′—C10	59.2 (18)
N1—Cd1—S4—P2	99.50 (19)	C8′—C9′—C10—C9	−98.7 (14)
S3—Cd1—S4—P2	−11.94 (11)	C8′—C9′—C10—C11′	−59.3 (18)
S1—Cd1—S4—P2	−147.72 (12)	C8′—C9′—C10—C11	1.0 (19)
S2—Cd1—S4—P2	−69.0 (4)	C8—C9—C10—C9′	42.1 (12)
Cd1—S2—P1—O1	110.3 (3)	C8—C9—C10—C11′	−94.0 (12)
Cd1—S2—P1—O2	−135.4 (3)	C8—C9—C10—C11	−63.7 (14)
Cd1—S2—P1—S1	−16.44 (16)	C9′—C10—C11—C12	−6.4 (18)
Cd1—S1—P1—O1	−108.9 (3)	C9—C10—C11—C12	62.6 (14)
Cd1—S1—P1—O2	142.3 (3)	C11′—C10—C11—C12	94.2 (13)
Cd1—S1—P1—S2	17.74 (17)	O2—C7—C12—C11	−175.8 (13)
Cd1—S4—P2—O4	−105.8 (3)	C8—C7—C12—C11	40 (2)
Cd1—S4—P2—O3	141.5 (3)	C12′—C7—C12—C11	−46.8 (12)
Cd1—S4—P2—S3	16.04 (15)	C8′—C7—C12—C11	91.8 (14)
Cd1—S3—P2—O4	107.8 (3)	C10—C11—C12—C7	−51.1 (18)
Cd1—S3—P2—O3	−145.1 (3)	C9′—C10—C11′—C12′	60.7 (17)
Cd1—S3—P2—S4	−17.73 (16)	C9—C10—C11′—C12′	102.6 (13)
O2—P1—O1—C1	−162.4 (7)	C11—C10—C11′—C12′	−41.8 (12)
S2—P1—O1—C1	−40.5 (7)	O2—C7—C12′—C11′	−171.7 (14)
S1—P1—O1—C1	87.2 (7)	C8—C7—C12′—C11′	−7.5 (18)
O1—P1—O2—C7	64.4 (9)	C12—C7—C12′—C11′	105.0 (14)
S2—P1—O2—C7	−55.6 (9)	C8′—C7—C12′—C11′	63.8 (17)
S1—P1—O2—C7	−179.6 (8)	C10—C11′—C12′—C7	−62.7 (18)
O4—P2—O3—C19	175.5 (6)	P2—O4—C13—C14	−84.2 (9)
S4—P2—O3—C19	−63.6 (7)	P2—O4—C13—C18	157.7 (7)
S3—P2—O3—C19	63.4 (7)	O4—C13—C14—C15	−177.3 (10)
O3—P2—O4—C13	86.3 (7)	C18—C13—C14—C15	−62.4 (12)
S4—P2—O4—C13	−34.4 (7)	C13—C14—C15—C16	56.4 (15)
S3—P2—O4—C13	−159.5 (6)	C14—C15—C16—C17	−52.5 (17)
S3—Cd1—N1—C26^{i}	−35.4 (13)	C15—C16—C17—C18	54.1 (17)
S1—Cd1—N1—C26^{i}	143.0 (13)	C16—C17—C18—C13	−57.7 (15)
S2—Cd1—N1—C26^{i}	64.1 (13)	O4—C13—C18—C17	−177.0 (9)
S4—Cd1—N1—C26^{i}	−113.4 (13)	C14—C13—C18—C17	62.9 (12)
S3—Cd1—N1—C25	143.3 (12)	P2—O3—C19—C24	132.8 (6)
S1—Cd1—N1—C25	−38.4 (12)	P2—O3—C19—C20	−106.5 (7)
S2—Cd1—N1—C25	−117.2 (12)	C24—C19—C20—C21	47.9 (14)
S4—Cd1—N1—C25	65.3 (12)	O3—C19—C20—C21	−63.8 (11)
S3—Cd1—N1—C26′^{i}	−165.2 (12)	C19—C20—C21—C22	−51.8 (14)
S1—Cd1—N1—C26′^{i}	13.2 (12)	C20—C21—C22—C23	58.2 (14)
S2—Cd1—N1—C26′^{i}	−65.7 (12)	C21—C22—C23—C24	−59.3 (14)
S4—Cd1—N1—C26′^{i}	116.8 (12)	C20—C19—C24—C23	−48.4 (14)
S3—Cd1—N1—C25′	13.5 (10)	O3—C19—C24—C23	69.7 (11)

S1—Cd1—N1—C25′	−168.1 (9)	C22—C23—C24—C19	53.7 (14)
S2—Cd1—N1—C25′	113.0 (9)	C26^{i}—N1—C25—C26	−1 (4)
S4—Cd1—N1—C25′	−64.5 (9)	C26′^{i}—N1—C25—C26	81 (2)
S3—Cd1—N1—C26"^{i}	89.6 (13)	C25′—N1—C25—C26	−52 (2)
S1—Cd1—N1—C26"^{i}	−92.1 (13)	C26"^{i}—N1—C25—C26	−80 (2)
S2—Cd1—N1—C26"^{i}	−170.9 (13)	C25"—N1—C25—C26	58 (2)
S4—Cd1—N1—C26"^{i}	11.6 (13)	Cd1—N1—C25—C26	−179.1 (16)
S3—Cd1—N1—C25"	−94.5 (10)	N1—C25—C26—N1^{i}	1 (3)
S1—Cd1—N1—C25"	83.8 (10)	C26^{i}—N1—C25′—C26′	−82.3 (19)
S2—Cd1—N1—C25"	4.9 (10)	C25—N1—C25′—C26′	49 (2)
S4—Cd1—N1—C25"	−172.5 (9)	C26′^{i}—N1—C25′—C26′	−4 (4)
P1—O1—C1—C2	153.9 (7)	C26"^{i}—N1—C25′—C26′	72.1 (18)
P1—O1—C1—C6	−87.8 (9)	C25"—N1—C25′—C26′	−66.5 (18)
O1—C1—C2—C3	−178.0 (8)	Cd1—N1—C25′—C26′	177.8 (14)
C6—C1—C2—C3	60.5 (11)	N1—C25′—C26′—N1^{i}	3 (3)
C1—C2—C3—C4	−61.8 (12)	C26^{i}—N1—C25"—C26"	72.5 (19)
C2—C3—C4—C5	55.6 (12)	C25—N1—C25"—C26"	−61 (2)
C3—C4—C5—C6	−61.6 (12)	C26′^{i}—N1—C25"—C26"	−80.2 (18)
C4—C5—C6—C1	61.8 (11)	C25′—N1—C25"—C26"	58.7 (19)
O1—C1—C6—C5	−174.0 (7)	C26"^{i}—N1—C25"—C26"	−11 (4)
C2—C1—C6—C5	−54.0 (9)	Cd1—N1—C25"—C26"	174.4 (15)
P1—O2—C7—C8	−104.2 (13)	N1—C25"—C26"—N1^{i}	8 (3)
P1—O2—C7—C12	112.9 (12)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.