

N2b—Zn1—S3c	104.5 (6)	N2—Zn2—N1a	93.9 (3)
N1b—Zn1—S3c	97.9 (5)	N2a—Zn2—N1a	77.2 (3)
S1—Zn1—S3c	120.5 (6)	O2w—Zn2—N1	167.1 (3)
S1—Zn1—S3Y	118.0 (6)	O1w—Zn2—N1	88.5 (2)
O2w—Zn2—O1w	87.4 (3)	N2—Zn2—N1	76.7 (3)
O2w—Zn2—N2	91.6 (3)	N2a—Zn2—N1	95.9 (3)
O1w—Zn2—N2	96.0 (2)	N1a—Zn2—N1	87.1 (3)

The structure was solved through a combination of direct methods and difference Fourier synthesis. Refinement was performed on F^2 using the whole data set. H atoms from coordinated water molecules were detected in a difference Fourier synthesis and subsequently refined with a rigid-body model. Those of the solvent water molecule could not be found. H atoms in the phen groups were included at their expected positions and allowed to ride on their host atoms. Fixed isotropic displacement parameters were used for all H atoms. One of the thiosulfate groups was found to be severely disordered and was refined as four different images of an idealized rigid group with occupancies constrained to sum to 1. The solvent water molecule was also found to be split in two positions. Lowering of the space-group symmetry did not result in a simpler model.

Data collection: *P3/P4-PC Diffractometer Program* (Siemens, 1991). Cell refinement: *P3/P4-PC Diffractometer Program*. Data reduction: *XDISK* in *SHELXTL/PC* (Sheldrick, 1990). Program(s) used to solve structure: *XS* in *SHELXTL/PC*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *XP* in *SHELXTL/PC*. Software used to prepare material for publication: *CIFTAB* in *SHELXL93* and *PARST* (Nardelli, 1983).

The authors would like to thank Fundación Andes for the purchase of the single-crystal diffractometer currently operating at the Universidad de Chile.

Lists of structure factors, anisotropic displacement parameters, least-squares-planes data, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: JZ1082). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The Five-Coordinate Cadmium Halide Bis(diethyldithiocarbamate) Complexes [PPh₄][Cd(S₂CNEt₂)₂Cl] and [PPh₄][Cd(S₂CNEt₂)₂Br]

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Abstract

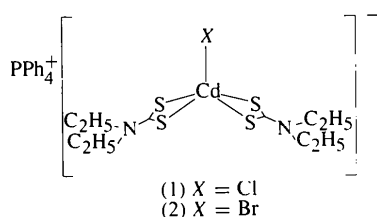
The title compounds, tetraphenylphosphonium chlorobis(diethyldithiocarbamate-*S,S*)cadmium(II), (C₂₄H₂₀P)-[CdCl(C₅H₁₀NS₂)₂], (1), and tetraphenylphosphonium bromobis(diethyldithiocarbamate-*S,S*)cadmium(II), (C₂₄-H₂₀P)[CdBr(C₅H₁₀NS₂)₂], (2), are isomorphous. The complexes are mononuclear with coordination spheres of the types S₄Cl and S₄Br, respectively. The central Cd atom is linked to four S atoms and two bidentate dithiocarbamate ligands and to the halide atom. The resulting Cd-atom coordination geometry is halfway between trigonal bipyramidal and square pyramidal. Principal dimensions include: Cd—S 2.573 (1)–2.682 (1) in (1) and 2.571 (3)–2.736 (2) Å in (2); Cd—Cl and Cd—Br 2.462 (1) and 2.626 (1) Å, respectively.

Comment

The characterization of mononuclear five-coordinate cadmium(II) compounds with sulfur ligation is of current interest with respect to structural and spectroscopic models for cadmium binding sites in biological molecules, particularly in a number of metallothioneins and metallo-regulatory proteins (Reddy, Zhang, Schlemper & Schrauzer, 1992, and references therein).

The reactions of the sulfur-bridged cadmium bis-(diethyldithiocarbamate) dimer with potentially monodentate anionic ligands to give the 1:1 adducts [Cd(S₂CNEt₂)₂X][−] (X = Cl, Br, I or NCS) have been reported recently (Baggio, Frigerio, Halac, Vega & Perec, 1992). The complexes were isolated as their [NEt₄]⁺ or [N^mBu₄]⁺ salts and characterized by elemental analysis and by spectroscopic techniques. In the

case of $[NEt_4][Cd(S_2CNEt_2)_2NCS]$, single crystals were obtained and the structure was determined by X-ray crystallography. The adduct was found to be mononuclear with a distorted CdS_4N nuclear core. Based on vibrational data the cadmium complexes with $X = Cl, Br$ and I also appeared to have five-coordinate mononuclear units, although on this basis alone the presence of sulfur- or halide-bridged coordination to give the more usual hexacoordinate Cd^{II} complexes could not be excluded. Herein we report the isolation of single crystals of $[PPh_4][Cd(S_2CNEt_2)_2Cl]$, (1), and $[PPh_4][Cd(S_2CNEt_2)_2Br]$, (2), and their structures as determined by X-ray crystallography.



The crystal data for (1) and (2) show that the complexes are isomorphous. Fig. 1 presents the structural diagram and the atomic numbering scheme for (1). Both anions have five-coordinate mononuclear CdS_4X units in which the metal atom is coordinated to four S atoms of two bidentate dithiocarbamate ligands and to the X atom of the halide ligand. Atoms S1, S4 and X ($X = Cl$ or Br) define the equatorial planes, and the Cd1 atoms are 0.0902 (4) in (1) and 0.0886 (6) Å in (2) below the corresponding planes pointing towards S3. The Cd1—S2 and Cd1—S3 axial bonds show average deviations of 20 (1) and 25 (1)° from the normal to the equatorial planes, which may be attributed to the acute bite angles of the spanning dithiocarbamate ligands [mean 67.85 (7) in (1) and 67.87 (6)° in (2)].

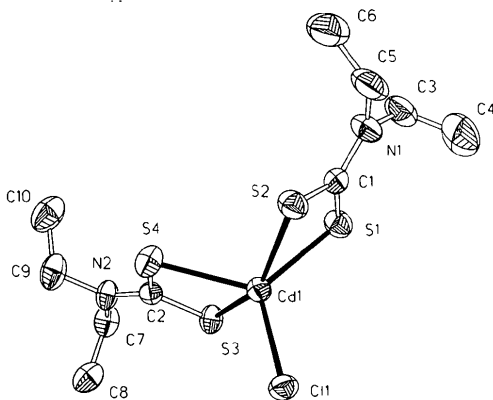


Fig. 1. View of $[Cd(S_2CNEt_2)_2Cl]^-$ in (1). H atoms have been omitted and displacement ellipsoids have been drawn at the 50% probability level.

The complexes exhibit a wide range of Cd—S bond lengths, with the equatorial Cd—S bonds significantly shorter than the axial bonds and with one bidentate ligand more asymmetrically bonded than the other [2.573 (1)–2.731 (1) and 2.615 (1)–2.682 (1) Å in (1) and 2.571 (3)–2.736 (2) and 2.617 (3)–2.685 (3) Å in (2), respectively]. The average (all bonds) Cd—S distance [2.65 (8) Å] is similar to the corresponding value in the related compound $[NEt_4][Cd(S_2CNEt_2)_2NCS]$ [2.61 (4) Å]. It thus appears that the nature of the halide does not significantly alter the Cd—S bond lengths in these five-coordinate complexes.

The terminal Cd—Cl and Cd—Br bond lengths are 2.462 (1) and 2.626 (1) Å, respectively, and are within the reported ranges for all terminal Cd—Cl and Cd—Br bonds (Orpen *et al.*, 1989). The dithiocarbamate ligands are almost planar with the small deviations being a twist about the S_2C-NR_2 bonds [2.5 (3) and 1.6 (3)° around C1—N1 and 1.1 (3) and 2.3 (3)° around C2—N2 for (1) and (2), respectively]. The distortion at the Cd atom may be conveniently described by the index parameter τ , defined as $[(S2-Cd1-S3) - (S4-Cd1-S1)]/60$ (Addison, Rao, Reedijk, Van Rijn & Vershooor, 1984). The calculated values of 0.50 for complexes (1) and (2) describe a type of structure which is 50% along the pathway of distortion from ideal square-pyramidal ($\tau = 0$) towards ideal trigonal-bipyramidal geometry ($\tau = 1$). The related compound $[NEt_4][Cd(S_2CNEt_2)_2NCS]$ shows a further distortion towards square-pyramidal geometry ($\tau = 0.27$). The coordination flexibility of five-coordinate Cd^{II} is well known (Bürgi, 1973) and undoubtedly reflects the d^{10} electron configuration of the metal ion, which rules out any ligand stabilizing effects in cadmium complexes.

Intermolecular distances in the reported complexes are larger than the corresponding sum of the van der Waals radii. Angles and other metric parameters of the ligands, as well as of the PPh_4^+ cations, can be regarded as unexceptional.

Experimental

All commercially available reagents and chemicals were of analytical or reagent-grade purity and used as received. Microanalyses were performed at INQUIMAE (Instituto de Química de Materiales, Medio Ambiente y Energía) with a Carlo Erba 1108 microanalyzer. Cadmium was analyzed by atomic absorption spectroscopy at the Analytical Laboratory of the Inorganic Chemistry Department. For (1), to a solution of $[PPh_4][Cl]$ (1.87 g, 0.005 mol) in acetone (200 cm^3) was slowly added solid $[Cd(S_2CNEt_2)_2]$ (2.05 g, 0.005 mol) at room temperature with constant stirring. The resulting mixture was filtered after 2 h and the filtrate evaporated *in vacuo* to ca 80 cm^3 . After addition of ca 40 cm^3 of light petroleum (b.p. 308–333 K), the solution was allowed to stand overnight at room temperature. The product separated as colourless crystals. Recrystallization was from light petroleum/acetone (1:1) at room temperature. Yield: 3.13 g, 80%. Analysis: found C

52.05, H 5.20, N 3.55, S 16.45, Cd 14.35%; C₃₄H₄₀CdClN₂PS₄ requires C 52.10, H 5.15, N 3.60, S 16.35, Cd 14.35%. Compound (2) was synthesized in an analogous manner from [PPh₄][Br] (2.10 g, 0.005 mol) and [Cd(S₂CNEt₂)₂] (2.05 g, 0.005 mol) in acetone–methylenechloride (3:1, 100 cm³). After stirring for 2 h, a light-yellow solution formed. It was filtered to remove traces of solids and allowed to stand at room temperature. After 24 h, light-yellow crystals were collected by vacuum filtration and dried under a nitrogen stream. Yield: 2.90 g, 70%. Analysis: found C 49.35, H 4.95, N 3.45, S 15.60, Cd 13.70%; C₃₄H₄₀BrCdN₂PS₄ requires C 49.30, H 4.90, N 3.40, S 15.50, Cd 13.60%.

Compound (1)

Crystal data

(C₂₄H₂₀P)[CdCl(C₅H₁₀NS₂)₂]

M_r = 783.74

Monoclinic

*P*2₁/*c*

a = 13.7460 (10) Å

b = 14.137 (2) Å

c = 19.039 (3) Å

β = 94.100 (10)°

V = 3690.3 (8) Å³

Z = 4

D_x = 1.411 Mg m⁻³

Data collection

Siemens R3m diffractometer

θ/2θ scans

Absorption correction:

ψ scan (XEMP in SHELXTL/PC; Sheldrick, 1991)

T_{min} = 0.729, *T_{max}* = 0.768

5096 measured reflections

4857 independent reflections

3509 observed reflections

[*I* > 2σ(*I*)]

Refinement

Refinement on *F*²

R[*F*² > 2σ(*F*²)] = 0.0358

wR(*F*²) = 0.0804

S = 1.036

4855 reflections

388 parameters

H atoms riding, C—H =

0.96 Å

w = 1/[σ²(*F_o*²) + (0.0331*P*)² + 0.9797*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (1)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i>
Cd1	0.21426 (2)	0.16757 (2)	0.68108 (2)	0.04625 (12)
Cl1	0.06421 (8)	0.15949 (9)	0.74410 (6)	0.0524 (3)
S1	0.32262 (10)	0.02007 (9)	0.67306 (7)	0.0573 (4)

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25

reflections

θ = 7.5–12.5°

μ = 0.959 mm⁻¹

T = 293 (2) K

Prismatic

0.28 × 0.24 × 0.22 mm

Colourless

R_{int} = 0.0217

θ_{max} = 22.54°

h = -14 → 14

k = 0 → 15

l = 0 → 20

2 standard reflections

monitored every 98

reflections

intensity decay: none

(Δ/σ)_{max} = -0.001

Δρ_{max} = 0.243 e Å⁻³

Δρ_{min} = -0.249 e Å⁻³

Extinction correction: none

Atomic scattering factors

from *International Tables*

for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

S2	0.35353 (9)	0.15654 (9)	0.79051 (7)	0.0562 (3)
S3	0.15193 (10)	0.19849 (8)	0.54630 (6)	0.0516 (3)
S4	0.26197 (10)	0.33605 (10)	0.63835 (6)	0.0580 (4)
N1	0.4767 (3)	0.0164 (3)	0.7662 (2)	0.0611 (12)
N2	0.1966 (3)	0.3722 (3)	0.5067 (2)	0.0523 (11)
C1	0.3928 (3)	0.0602 (3)	0.7453 (2)	0.0482 (12)
C2	0.2026 (3)	0.3092 (3)	0.5585 (2)	0.0412 (11)
C3	0.5107 (4)	-0.0675 (4)	0.7294 (3)	0.079 (2)
C4	0.4694 (5)	-0.1547 (5)	0.7584 (4)	0.121 (3)
C5	0.5381 (4)	0.0445 (4)	0.8284 (3)	0.083 (2)
C6	0.6252 (5)	0.1001 (5)	0.8105 (4)	0.113 (3)
C7	0.1428 (4)	0.3562 (4)	0.4386 (2)	0.0614 (15)
C8	0.0395 (4)	0.3921 (4)	0.4374 (3)	0.075 (2)
C9	0.2406 (4)	0.4672 (4)	0.5147 (3)	0.069 (2)
C10	0.3428 (4)	0.4704 (5)	0.4922 (3)	0.095 (2)
P1	0.76323 (8)	0.15951 (8)	0.55021 (6)	0.0373 (3)
C11	0.6347 (3)	0.1724 (3)	0.5290 (2)	0.0402 (11)
C12	0.5969 (4)	0.1950 (4)	0.4621 (3)	0.0620 (15)
C13	0.4976 (4)	0.2123 (5)	0.4505 (3)	0.081 (2)
C14	0.4381 (4)	0.2058 (4)	0.5044 (4)	0.078 (2)
C15	0.4742 (4)	0.1812 (4)	0.5698 (3)	0.079 (2)
C16	0.5723 (4)	0.1634 (4)	0.5826 (3)	0.0634 (14)
C21	0.8283 (3)	0.1447 (3)	0.4732 (2)	0.0417 (12)
C22	0.8331 (4)	0.2204 (4)	0.4271 (3)	0.0596 (14)
C23	0.8822 (4)	0.2114 (5)	0.3668 (3)	0.077 (2)
C24	0.9284 (4)	0.1282 (6)	0.3533 (3)	0.082 (2)
C25	0.9256 (4)	0.0546 (5)	0.3987 (3)	0.078 (2)
C26	0.8750 (3)	0.0607 (4)	0.4588 (3)	0.0557 (14)
C31	0.7810 (3)	0.0596 (3)	0.6071 (2)	0.0397 (11)
C32	0.7384 (4)	-0.0261 (4)	0.5878 (3)	0.0605 (14)
C33	0.7521 (4)	-0.1048 (4)	0.6292 (3)	0.069 (2)
C34	0.8112 (4)	-0.0983 (4)	0.6908 (3)	0.068 (2)
C35	0.8534 (4)	-0.0140 (4)	0.7110 (3)	0.067 (2)
C36	0.8394 (4)	0.0653 (4)	0.6689 (3)	0.0534 (13)
C41	0.8087 (3)	0.2638 (3)	0.5944 (2)	0.0358 (11)
C42	0.7476 (4)	0.3275 (3)	0.6247 (2)	0.0541 (13)
C43	0.7868 (5)	0.4044 (4)	0.6615 (3)	0.066 (2)
C44	0.8861 (5)	0.4184 (4)	0.6686 (3)	0.0609 (15)
C45	0.9466 (4)	0.3566 (3)	0.6383 (3)	0.0575 (14)
C46	0.9086 (4)	0.2790 (3)	0.6015 (2)	0.0507 (13)

Table 2. Selected geometric parameters (Å, °) for (1)

Cd1—Cl1	2.4619 (12)	S2—C1	1.718 (5)
Cd1—S1	2.5734 (13)	S3—C2	1.722 (4)
Cd1—S4	2.6155 (14)	S4—C2	1.716 (4)
Cd1—S3	2.6823 (13)	N1—C1	1.343 (6)
Cd1—S2	2.7313 (13)	N2—C2	1.327 (5)
S1—C1	1.719 (5)		
Cl1—Cd1—S1	120.00 (4)	C1—S1—Cd1	88.8 (2)
Cl1—Cd1—S4	115.55 (4)	C1—S2—Cd1	83.8 (2)
S1—Cd1—S4	124.08 (5)	C2—S3—Cd1	85.5 (2)
Cl1—Cd1—S3	104.62 (4)	C2—S4—Cd1	87.7 (2)
S1—Cd1—S3	102.82 (4)	N1—C1—S2	120.7 (4)
S4—Cd1—S3	67.92 (4)	N1—C1—S1	120.3 (4)
Cl1—Cd1—S2	101.04 (4)	S2—C1—S1	118.9 (3)
S1—Cd1—S2	67.78 (4)	N2—C2—S4	120.7 (3)
S4—Cd1—S2	96.41 (4)	N2—C2—S3	120.5 (3)
S3—Cd1—S2	153.84 (4)	S4—C2—S3	118.8 (3)

Compound (2)

Crystal data

(C₂₄H₂₀P)[CdBr(C₅H₁₀NS₂)₂]

M_r = 828.2

Monoclinic

*P*2₁/*c*

a = 13.858 (2) Å

b = 14.159 (3) Å

c = 19.250 (3) Å

β = 93.87°

V = 3768.5 (11) Å³

Z = 4

D_x = 1.460 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25

reflections

θ = 7.5–12.5°

μ = 1.929 mm⁻¹

T = 293 (2) K

Polyhedron

0.22 × 0.18 × 0.14 mm

Light yellow

Data collection

Siemens R3m diffractometer
 $\omega/2\theta$ scans
 Absorption correction:
 ψ scan (XEMP in
 SHELXTL/PC; Sheldrick,
 1991)
 $T_{\min} = 0.677$, $T_{\max} =$
 0.791
 5646 measured reflections
 4944 independent reflections
 3337 observed reflections
 $[I > 2\sigma(I)]$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.0567$
 $wR(F^2) = 0.1508$
 $S = 1.072$
 4944 reflections
 388 parameters
 H atoms riding, C—H
 0.96 Å
 $w = 1/[\sigma^2(F_o^2) + (0.0594P)^2$
 $+ 11.2259P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$R_{\text{int}} = 0.0397$
 $\theta_{\text{max}} = 22.55^\circ$
 $h = -14 \rightarrow 14$
 $k = -1 \rightarrow 15$
 $l = 0 \rightarrow 20$
 2 standard reflections
 monitored every 98
 reflections
 intensity decay: none

$(\Delta/\sigma)_{\text{max}} = -0.001$
 $\Delta\rho_{\text{max}} = 0.533 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -1.060 \text{ e } \text{Å}^{-3}$
 Extinction correction: none
 Atomic scattering factors
 from *International Tables*
 for *Crystallography* (1992,
 Vol. C, Tables 4.2.6.8 and
 6.1.1.4)

C41	0.8090 (6)	0.2620 (6)	0.5925 (4)	0.038 (2)
C42	0.7488 (7)	0.3247 (7)	0.6245 (5)	0.056 (2)
C43	0.7877 (9)	0.4023 (7)	0.6606 (5)	0.068 (3)
C44	0.8872 (9)	0.4155 (7)	0.6660 (5)	0.063 (3)
C45	0.9464 (8)	0.3548 (7)	0.6352 (5)	0.063 (3)
C46	0.9065 (7)	0.2771 (6)	0.5976 (5)	0.056 (3)

Table 4. Selected geometric parameters (Å, °) for (2)

Cd1—S1	2.571 (3)	S2—C1	1.717 (9)
Cd1—S4	2.617 (3)	S3—C2	1.721 (9)
Cd1—Br1	2.6260 (13)	S4—C2	1.735 (9)
Cd1—S3	2.685 (3)	N1—C1	1.323 (11)
Cd1—S2	2.736 (2)	N2—C2	1.306 (11)
S1—C1	1.734 (9)		
S1—Cd1—S4	124.90 (9)	C1—S1—Cd1	89.1 (3)
S1—Cd1—Br1	119.87 (7)	C1—S2—Cd1	84.1 (3)
S4—Cd1—Br1	114.89 (7)	C2—S3—Cd1	86.0 (3)
S1—Cd1—S3	103.46 (8)	C2—S4—Cd1	87.9 (3)
S4—Cd1—S3	67.93 (7)	N1—C1—S2	121.6 (7)
Br1—Cd1—S3	103.78 (6)	N1—C1—S1	120.1 (7)
S1—Cd1—S2	67.81 (8)	S2—C1—S1	118.3 (5)
S4—Cd1—S2	97.01 (8)	N2—C2—S3	121.6 (7)
Br1—Cd1—S2	100.85 (7)	N2—C2—S4	120.3 (7)
S3—Cd1—S2	154.85 (9)	S3—C2—S4	118.1 (5)

Systematic absences ($0k0, k = 2n; h0l, l = 2n$) indicated $P2_1/c$ as the space group for both compounds.

For both compounds, data collection: *P3/P4-PC Diffractometer Program* (Siemens, 1991); cell refinement: *P3/P4-PC Diffractometer Program*; data reduction: *XDISK* in *SHELXTL/PC* (Sheldrick, 1991); program(s) used to solve structures: *XS* in *SHELXTL/PC*; program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993); molecular graphics: *XP* in *SHELXTL/PC*; software used to prepare material for publication: *CIFTAB* in *SHELXL93* and *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1103). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 3. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (2)

	x	y	z	U_{eq}
Cd1	0.2194 (5)	0.16902 (5)	0.68054 (3)	0.0488 (2)
Br1	0.05975 (8)	0.16172 (8)	0.74647 (6)	0.0708 (3)
P1	0.7619 (2)	0.1581 (2)	0.54924 (12)	0.0416 (6)
S1	0.3259 (2)	0.0211 (2)	0.67367 (13)	0.0607 (7)
S2	0.3559 (2)	0.1577 (2)	0.78969 (14)	0.0608 (7)
S3	0.1566 (2)	0.1997 (2)	0.54742 (12)	0.0541 (6)
S4	0.2659 (2)	0.3375 (2)	0.63789 (12)	0.0617 (7)
N1	0.4763 (6)	0.0163 (6)	0.7668 (5)	0.068 (2)
N2	0.2001 (6)	0.3731 (5)	0.5083 (4)	0.054 (2)
C1	0.3956 (6)	0.0610 (6)	0.7459 (5)	0.049 (2)
C2	0.2059 (6)	0.3106 (6)	0.5583 (4)	0.047 (2)
C3	0.5090 (8)	-0.0705 (9)	0.7308 (6)	0.083 (4)
C4	0.4655 (10)	-0.1564 (9)	0.7618 (9)	0.125 (6)
C5	0.5376 (8)	0.0429 (9)	0.8287 (6)	0.081 (4)
C6	0.6242 (9)	0.1010 (10)	0.8116 (8)	0.120 (5)
C7	0.1448 (8)	0.3561 (7)	0.4413 (5)	0.069 (3)
C8	0.0421 (8)	0.3907 (9)	0.4411 (6)	0.084 (4)
C9	0.2426 (8)	0.4680 (7)	0.5165 (6)	0.073 (3)
C10	0.3434 (9)	0.4714 (9)	0.4925 (6)	0.094 (4)
C11	0.6338 (6)	0.1721 (6)	0.5275 (5)	0.048 (2)
C12	0.5980 (7)	0.1961 (8)	0.4620 (6)	0.068 (3)
C13	0.5000 (8)	0.2143 (9)	0.4503 (6)	0.084 (4)
C14	0.4395 (8)	0.2079 (9)	0.5028 (8)	0.085 (4)
C15	0.4755 (8)	0.1820 (9)	0.5674 (8)	0.087 (4)
C16	0.5721 (7)	0.1632 (8)	0.5808 (6)	0.071 (3)
C21	0.8274 (6)	0.1422 (6)	0.4725 (4)	0.043 (2)
C22	0.8323 (7)	0.2165 (7)	0.4271 (5)	0.063 (3)
C23	0.8825 (8)	0.2066 (10)	0.3673 (6)	0.081 (4)
C24	0.9291 (9)	0.1230 (12)	0.3557 (6)	0.087 (4)
C25	0.9229 (8)	0.0501 (10)	0.3999 (7)	0.083 (4)
C26	0.8726 (7)	0.0584 (7)	0.4588 (5)	0.060 (3)
C31	0.7776 (6)	0.0584 (6)	0.6060 (4)	0.043 (2)
C32	0.7348 (8)	-0.0267 (7)	0.5870 (6)	0.071 (3)
C33	0.7494 (9)	-0.1048 (8)	0.6294 (7)	0.078 (3)
C34	0.8054 (9)	-0.0985 (8)	0.6895 (7)	0.077 (3)
C35	0.8485 (9)	-0.0149 (9)	0.7094 (6)	0.084 (3)
C36	0.8337 (7)	0.0653 (7)	0.6671 (5)	0.059 (3)