$[Ni(C_5H_8NOS_2)(C_{26}H_{24}P_2)]ClO_4.CH_2Cl_2$

C27—N28A	1.351 (13)	Cl3—O4	1.35 (2)
C27—N28B	1.347 (13)	Cl3—O1A	1.253 (10)
N28A—C29A	1.49 (2)	C13—O2A	1.304 (13)
N28A-C33A	1.48 (2)	C13—O3A	1.333 (14)
C29A—C30A	1.51 (2)	C13O4A	1.41 (2)
C30A—O31A	1.48 (5)		
P1—Ni—P2	86.81 (4)	N28A—C29A—C30A	110.0 (9)
P1—Ni—S1	102.69 (4)	O31A-C30A-C29A	109.8 (18)
P2—Ni—S2	93.93 (4)	C32A—O31A—C30A	110 (3)
\$1Ni\$2	79.36 (4)	O31A—C32A—C33A	113.2 (15)
C27—S1—Ni	84.51 (14)	N28A—C33A—C32A	109.4 (10)
C27—S2—Ni	85.21 (14)	C27—N28B—C29B	122.7 (11)
C3-P1-C9	104.1 (2)	C27—N28B—C33B	123.7 (10)
C3-P1-C2	105.3 (2)	C33BN28BC29B	113.5 (10)
C9—P1—C2	107.1 (2)	N28B—C29B—C30B	109.9 (9)
C3—P1—Ni	104.67 (13)	O31B—C30B—C29B	107.7 (22)
C9-P1-Ni	125.41 (14)	C32B-O31B-C30B	113 (3)
C2—P1—Ni	108.54 (13)	O31B-C32B-C33B	112.0 (20)
C15—P2—C21	107.4 (2)	N28BC33BC32B	109.7 (10)
C15—P2—C1	107.8 (2)	CI1-C34-C12	114.6 (4)
C21—P2—C1	107.1 (2)	01—Cl3—O2	91.8 (13)
C15—P2—Ni	115.30 (13)	O1—C13—O3	115.9 (18)
C21-P2-Ni	109.00 (14)	01-Cl3-04	124.8 (14)
C1—P2—Ni	109.92 (13)	O2—C13—O3	104.9 (14)
N28 <i>B</i> —C27—S2	123.4 (6)	O2-C13-O4	108.5 (17)
N28A—C27—S2	122.4 (6)	O3-C13-O4	107.8 (19)
N28B—C27—S1	123.5 (6)	O1A-Cl3-O2A	128.8 (14)
N28A—C27—S1	123.7 (6)	01A-Cl3-O3A	84.5 (15)
S2-C27-S1	110.8 (2)	01A-C13-O4A	113.6 (14)
C27—N28A—C29A	123.8 (10)	02A-C13-O3A	107.2 (17)
C27—N28A—C33A	122.1 (10)	02A-Cl3-O4A	112.5 (16)
C33A—N28A—C29A	112.4 (10)	O3A-Cl3-O4A	101.0 (11)

Data collection, cell refinement and data reduction were performed using XSCANS (Siemens, 1991). The structure was solved by direct methods using SHELXS86 (Sheldrick, 1990a) and refined using SHELXL93 (Sheldrick, 1993). Atoms in the morpholine ring showed very high disorder with unreliable C-C bond lengths (1.12 Å). Moreover, the displacement ellipsoids for all the atoms in the ring were oriented in the same direction, *i.e.* perpendicular to the mean plane of the ring. Hence, it was decided to consider the morpholine ring as two entities with opposite orientations (A and B) and the occupancies of A and B were initially refined and then fixed at 0.5. The atoms in A and B were refined anisotropically with the same U_{ij} values being assigned to the same atom species $(N28A \equiv N28B, O31A \equiv O31B, CnA \equiv CnB)$. The O atoms of the disordered perchlorate group were divided into two sets, each having 0.5 occupancy, and refined anisotropically. The H atoms were fixed geometrically and not refined, but were allowed to ride on those atoms to which they are attached. SHELXTL/PC (Sheldrick, 1990b) software was used for the molecular graphics and PARST (Nardelli, 1983) was used for all other geometrical calculations.

One of the authors (KC) thanks Universiti Sains Malaysia for a Visiting Post Doctoral Research Fellowship.

Lists of structure factors, anisotropic displacement parameters, Hatom coordinates and complete geometry have been deposited with the IUCr (Reference: LI1125). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Aravamudan, G., Brown, D. H. & Venkappayya, D. (1971). J. Chem. Soc. A, pp. 2744–2747.

© 1995 International Union of Crystallography Printed in Great Britain – all rights reserved Butcher, R. J. & Sinn, E. (1975). J. Chem. Soc. Dalton Trans. pp. 2517-2522.

- Butcher, R. J. & Sinn, E. (1976). J. Am. Chem. Soc. 98, 2440-2449,
- Esperas, S. & Husebye, S. (1975). Acta Chem. Scand. Ser. A, 29, 185-194.
- Gabor, B., Krüger, C., Marczinke, B., Mynott, R. & Wilke, G. (1991). Angew. Chem. Int. Ed. Engl. 30, 1666–1668.
- Healy, P. C. & Sinn, E. (1974). Inorg. Chem. 14, 109-115.
- Nardelli, M. (1983). Comput. Chem. 7, 95-98.
- Ramalingam, K., Aravamudan, G. & Seshasayee, M. (1987). Inorg. Chim. Acta. 128, 231-237.
- Ramalingam, K., Aravamudan, G., Seshasayee, M. & Subramanyam, Ch. (1984). Acta Cryst. C40, 965–967.
- Sheldrick, G. M. (1990). Acta Cryst. A46, 467-473.
- Sheldrick, G. M. (1990a). Acta Cryst. A46, 467-473.
- Sheldrick, G. M. (1990b). SHELXTL/PC Users Manual. Siemens
- Sheldrick, G. M. (1993). SHELXL93. Program for Crystal Structure Refinement. Univ. of Göttingen, Germany.
- Siemens (1991). XSCANS Users Manual. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Stahl, K. (1983a). Acta Cryst. B39, 612-620.
- Stahl, K. (1983b). Inorg. Chim. Acta, 75, 85-91.

Acta Cryst. (1995). C51, 370-374

fac-[Co(C₅H₄NOS)₃].H₂O. $\frac{1}{2}$ CH₃OH and fac-[Co(C₅H₄NOS)₃]. $\frac{1}{3}$ CH₃OH

Yong-Jin Xu, Bei-Sheng Kang,* Xue-Tai Chen and Liang-Reng Huang

State Key Laboratory of Structural Chemistry and Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China

(Received 23 September 1993; accepted 1 June 1994)

Abstract

Crystals of tris(2-mercaptopyridine N-oxido)cobalt-(III) monohydrate hemimethanol solvate, fac- $[Co(C_5H_4NOS)_3]$.H₂O. $\frac{1}{2}CH_3OH$ (1), contain fac- $[Co(III)(mpo)_3]$ (Hmpo = 2-mercaptopyridine Noxide), H₂O and MeOH molecules linked by hydrogen bonds. The asymmetric unit consists of two molecules of the cobalt complex, two water and one methanol molecule. The asymmetric unit of the closely related complex tris(2-mercaptopyridine *N*-oxido)cobalt(III) ¹/₃-methanol solvate, fac- $[Co(C_5H_4NOS)_3]_3CH_3OH$ (2), contains three discrete Co(mpo)₃ molecules and one MeOH molecule which is linked to one of the Co(mpo)₃ units via a hydrogen bond. The Co^{III} complex molecules in (1) and (2) do not differ significantly. Each Co atom is coordinated by an O₃S₃ donor set which defines a distorted facial octahedron. Three mpo ligands are chelated to each Co atom, the average O-Co-S

bite angle is 87.5 (2) for (1) and 87.4 (2)° for (2). The average Co—S and Co—O distances are 2.205 (3) and 1.942 (2) Å, respectively, for (1), and 2.205 (3) and 1.951 (5) Å, respectively, for (2).

Comment

Both compounds (1) and (2) were synthesized as part of our investigation of transition metal complexes with bidentate sulfur-oxygen ligands (Kang, Weng, Wu, Wang, Guo, Huang, Huang & Liu, 1988; Chen, Hu, Weng, Xu, Wu & Kang, 1991). Seven chelating modes for the ligand o-mercaptophenol (H_2mp) have been observed in a series of mixed O,S-ligated transition metal complexes (Kang, Weng, Liu, Wu,



Fig. 1. Structure and atomic labelling of (1) with displacement ellipsoids drawn at the 40% probability level (*ORTEPII*; Johnson, 1976).

Huang, Lu, Cai, Chen & Lu, 1990; Kang, Peng, Hong, Wu, Chen, Weng, Lei & Liu, 1991; Kang, Hu, Weng, Wu, Chen & Xu, 1992). We have now extended our research to the ligand 2-mercaptopyridine *N*-oxide (Hmpo).



The structures of the Co(mpo)₃ units of both compounds are quite similar to those reported earlier for fac-[Co(mpo)₃].MeCN (Hu, Weng, Huang, Chen, Wu & Kang, 1991) although the average Co-S, Co-O and S-C distances in (1) and (2) are all lengthened slightly (by nearly 0.01 Å) as a result of the presence of hydrogen bonds and also of differences in the molecular packing. The average O-N distances are within the range found for other mpoligated complexes (Kang, Xu, Peng, Wu, Chen, Hu, Hong & Lu, 1993). In compound (1), the ligand atoms O(4) and O(6) are connected to $H_2O(w)$ and the atom O(5) to $H_2O(ww)$ via weak hydrogen bonds, while the latter water molecule $[H_2O(ww)]$ is also hydrogen bonded to $H_2O(w)$ and MeO(1m)H. The mean chelate angles Co-S-C and Co-O-N $[96.4(2) \text{ and } 115.8(2)^{\circ}, \text{ respectively, for (1), and}$ 97.1 (2) and 115.8 (2)°, respectively, for (2)] and the mean bite angle of 87.5 (2) in (1) and 87.4 (2) $^{\circ}$ in (2) are very close to those reported by Kang, Xu, Peng,



Fig. 2. Structure and atomic labelling of (2) with displacement ellipsoids drawn at the 40% probability level (ORTEPII; Johnson, 1976).

Wu, Chen, Hu, Hong & Lu (1993), and correspond well to the previous interpretation of bonding orbitals. The packing of the molecules of (2) in the unit cell is interesting, consisting of two sets of staircaselike stripes made up of parallel and independent triangular units of three Co(mpo)₃ groups with one MeOH tail (via a hydrogen bond). This type of arrangement of molecular units may lead to interesting physical properties which are still under investigation. Figs. 1 and 2 show the asymmetric units of (1) and (2), respectively.

Experimental

Crystals of (1) were obtained from the reaction of CoCl₂ with mpoNa (1:2 ratio) in MeOH solvent (AR, 0.5% water) at room temperature, while those of (2) came from the reaction of CoCl₂ with mpoNa (1:2 ratio) in anhydrous MeOH (dried vigorously before use) at room temperature.

Compound (1)

Crystal data

refined

$[Co(C_{5}H_{4}NOS)_{3}].H_{2}O\frac{1}{2}CH_{4}O$ $M_{r} = 471.44$ Triclinic $P\overline{1}$ a = 12.679 (6) Å b = 14.794 (10) Å c = 12.653 (7) Å $\alpha = 114.16$ (5)° $\beta = 117.54$ (4)° $\gamma = 75.97$ (6)° V = 1915.9 Å ³ Z = 4 $D_{x} = 1.63$ Mg m ⁻³	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å Cell parameters from 20 reflections $\theta = 9-12^{\circ}$ $\mu = 1.24 \text{ mm}^{-1}$ T = 293 K Cube $0.30 \times 0.25 \times 0.20 \text{ mm}$ Black
Data collection Rigaku AFC-5 <i>R</i> diffractom- eter $\omega - 2\theta$ scans Absorption correction: empirical $T_{min} = 0.901, T_{max} = 0.996$ 7088 measured reflections 6944 independent reflections 2728 observed reflections $[I > 2\sigma(I)]$	$R_{int} = 0.082$ $\theta_{max} = 25^{\circ}$ $h = 0 \rightarrow 15$ $k = -17 \rightarrow 17$ $l = -15 \rightarrow 13$ 3 standard reflections monitored every 250 reflections intensity decay: 0.8%
Refinement Refinement on F R = 0.062 wR = 0.064 S = 1.36 2584 reflections 487 parameters H-atom parameters not	$w = 4F_o^2/\sigma^2(F_o^2)$ $(\Delta/\sigma)_{max} = 0.42$ $\Delta\rho_{max} = 0.65 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{min} = -0.52 \text{ e } \text{\AA}^{-3}$ Extinction correction: none Atomic scattering factors from Cromer & Waber

Compound (2)

Crystal data	
$[Co(C_5H_4NOS)_3].\frac{1}{3}CH_4O$ $M_r = 448.08$ Monoclinic $P2_1/n$ a = 21.997 (11) Å	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å Cell parameters from 20 reflections $\theta = 9-12^{\circ}$
b = 9.094 (5) Å c = 27.594 (9) Å $\beta = 95.87 (4)^{\circ}$ $V = 5490.8 \text{ Å}^{3}$ Z = 12 $D_{x} = 1.63 \text{ Mg m}^{-3}$	$\mu = 1.24 \text{ mm}^{-1}$ T = 296 (1) K Cubes $0.41 \times 0.33 \times 0.24 \text{ mm}$ Black

Data collection

(1974)

Rigaku AFC-5R diffractom- eter	5535 observed reflections $[I > 3\sigma(I)]$
ω -2 θ scans	$R_{\rm int} = 0.046$
Absorption correction:	$\theta_{\rm max} = 25^{\circ}$
empirical	$h = 0 \rightarrow 26$
$T_{\min} = 0.810, T_{\max} =$	$k = 0 \rightarrow 10$
1.00	$l = -32 \rightarrow 32$
10 629 measured reflections	3 standard reflections
10 614 independent	monitored every 250
reflections	reflections
	intensity decay: 0.4%

Refinement

Refinement on F R = 0.052wR = 0.062S = 1.385523 reflections 694 parameters H-atom parameters not refined

: 0.4% $w = 1/[\sigma^2(F_o^2) + (0.010F_o)^2]$ +1] $(\Delta/\sigma)_{\rm max} = 0.03$ $\Delta \rho_{\rm max} = 0.44 \ {\rm e} \ {\rm \AA}^{-3}$ $\Delta \rho_{\rm min} = -0.57 \ {\rm e} \ {\rm \AA}^{-3}$ Extinction correction: none Atomic scattering factors

from Cromer & Waber

(1974)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters $(Å^2)$ for (1)

$$B_{\rm eq} = (4/3) \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	у	Z	Beq
Co(1)	0.4826(1)	0.7273 (1)	0.3470(1)	2.61 (4
Co(2)	0.1697 (1)	0.7858(1)	0.7138(1)	2.74 (4
S(1)	0.5732 (3)	0.7724 (2)	0.2659 (3)	3.80 (9
S(2)	0.3152 (3)	0.7950 (2)	0.9017 (3)	3.54 (8
S(3)	0.0415 (3)	0.7515 (2)	0.7621 (3)	3.50 (9
S(4)	0.1180 (3)	0.9463 (2)	0.7803 (3)	3.43 (9
S(5)	0.4449 (3)	0.8838 (2)	0.4484 (3)	3.45 (9
S(6)	0.6502 (3)	0.7203 (2)	0.5128 (3)	3.64 (9
O(w)	0.1568 (9)	0.7169 (8)	0.3644 (9)	7.9 (4)
O(ww)	0.139 (2)	0.606 (2)	0.129 (2)	14 (1)
O(1)	0.5089 (6)	0.5907 (5)	0.2463 (6)	3.2 (2)
O(1 <i>m</i>)	-0.089 (2)	0.665 (3)	-0.0221 (2)	19 (1)
O(2)	0.2870 (6)	0.8087 (5)	0.6705 (6)	3.2 (2)
C(2m)	-0.097 (3)	0.736 (3)	0.084 (4)	15 (2)
O(3)	0.1984 (6)	0.6444 (5)	0.6393 (6)	3.5 (2)
O(4)	0.0516 (7)	0.7803 (5)	0.5447 (6)	3.9 (2)
O(5)	0.3275 (6)	0.7341 (5)	0.2097 (6)	3.4 (2)
O(6)	0.4054 (6)	0.6767 (5)	0.4114 (6)	3.6 (2)

Table 3. Fractional atomic coordinates and equivalent

N(1) 0.3919 (7) 0.373 (6) 0.769 (7) 1.21 (2) isotropic displacement parameters (Å ³) for (2) N(3) 0.2323 (7) 0.2323 (6) 0.2311 (7) 2.4 (2) $B_{eq} = (4/3)\Sigma_{c} \Sigma_{c} \beta_{c} h_{c} h_{c} + J_{c} + J_{c} h_{c} + J_{c} + J_{c} h_{c} + J_{c} + J_{c} + J_{c} h_{c} + J_{c} + J_{c} + J_{c} h_{c} + J_{c} + J_{c}$	N(11)	0.5769 (7)	0.5755 (6)) 0.1848 (7)	2.8 (2)	Table 3	. Fractional	atomic coor	dinates and	equivale
$ \begin{array}{c} \mathbf{R}_{(11)} & 0.138(3) & 0.324.10 & 0.931(1) & 14(3) & \mathbf{R}_{(21)} & \mathbf{R}_{(21$	N(21)	0.3919 (7)	0.8373 (6) 0.7669 (7)	2.5 (2)	iso	tropic displa	acement parar	neters (Ų) fe	or (2)
$ \begin{array}{c} n(3) & -0.232 (n) & 0.236 (n) & 0.211 (r) & 2.9 (1) \\ n(3) & 0.236 (n) & 0.236 (n) & 0.211 (r) & 2.9 (1) \\ n(4) & 0.238 (n) & 0.236 (n) & 0.217 (n) & 3.4 (n) \\ n(4) & 0.038 (n) & 0.238 (n) & 0.237 (n) & 3.4 (n) \\ n(4) & 0.036 (n) & 0.238 (n) & 0.237 (n) & 0.345 (n) \\ n(4) & 0.036 (n) & 0.238 (n) & 0.238 (n) \\ n(4) & 0.036 (n) & 0.238 (n) & 0.112 (n) & 5.9 (n) & 0.12 (n) & 0.238 (n) & 0.238 (n) \\ n(4) & 0.036 (n) & 0.238 (n) & 0.112 (n) & 5.9 (n) & 0.12 (n) & 0.497 (n) & 0.238 (n) \\ n(4) & 0.036 (n) & 0.238 (n) & 0.112 (n) & 5.6 (n) & 1.2 (n) & 0.497 (n) & 0.0488 (n) & 0.0388 (n) \\ n(2) & 0.233 (n) & 0.238 (n) & 0.121 (n) & 5.6 (n) & 1.2 (n) & 0.448 (n) & 0.0488 (n) & 0.488 (n) & 4.06 (n) \\ n(2) & 0.036 (n) & 0.036 (n) & 0.597 (n) & 5.6 (n) & 5.6 (n) & 0.038 (n) & 0.0388 (n) & 0.466 (n) \\ n(2) & 0.036 (n) & 0.0378 (n) & 5.6 (n) & 5.6 (n) & 5.2 (n) & 0.038 (n) & 0.0483 (n) & 3.4 (n) & 0.6 (n) & 0.038 (n) & 0.037 (n) & 0.066 (n) & 1.4 (n) & 5.2 (n) & 0.038 (n) & 0.038 (n) & 0.038 (n) & 0.037 (n) & 0.066 (n) & 0.459 (n) & 0.12 (n) & 0.038 (n) & 0.038 (n) & 0.037 (n) & 0.066 (n) & 0.459 (n) & 0.038 (n) & 0.037 (n) & 0.066 (n) & 0.459 (n) & 0.038 (n) & 0.037 (n) & 0.048 (n) & 0.043 (n) & 0.038 (n) & 0.037 (n) & 0.048 (n) & 0.038 (n) & 0.037 (n) & 0.008 (n) & 0.031 (n) & 0.037 (n) & 0.008 (n) & 0.031 (n) & 0.037 (n) & 0.038 (n) & 0.037 (n) & 0.008 (n) & 0.50 (n) & 0.001 (n) & 0.037 (n) & 0.038 (n) & 0.037 (n) & 0.003 (n) & 0.007 (n) & 0.001 (n) & 0.037 (n) & 0.038 (n) $	N(31)	0.1438 (8)	0.5842 (6) 0.6491 (/)) 0.5381 (7)	2.8(3) 34(3)		nepre unipre		, , , , , , , , , , , , , , , , , , ,	
$ \begin{array}{c} \mathbf{x} (a) \\ \mathbf{x} (b) \\ \mathbf{x} (c) \\ x$	N(41) N(51)	-0.0180(8) 0.2823(7)	0.8049 (0	0.2151(7)	2.9(2)		Be	$_{q} = (4/3) \Sigma_{i} \Sigma_{j} \beta_{i}$	ij a i.aj.	
$ \begin{array}{c} c_{12} \\ c_{13} \\ c_{13} \\ c_{14} \\ c_{14} \\ c_{16} \\ c_{1$	N(61)	0.4782 (8)	0.6535 (6) 0.5174 (7)	2.9 (3)		x	ν	z	Bea
$ \begin{array}{c} C(13) & 0.672 (10) & 0.493 (10) & 0.493 (10) & 49 (4) & C_{0}(2) & 1.02291 (5) & -0.1179 (1) & 0.8897 (4) & 228 (2) \\ C(14) & 0.056 (10) & 0.514 (10) & 0.0451 (10) & 0.416 (10) & 0.410 & 0.271 (2) \\ 0.0570 (10) & 0.0514 (10) & 0.0514 (10) & 0.1810 (10) & 1.61 (2) & S(11) & 0.0256 (1) & 0.1273 (1) & 0.6198 (6) & 1.310 (2) \\ C(22) & 0.420 (10) & 0.852 (10) & 0.545 (10) & 0.54 (1) & 0.513 (1) & 0.0256 (1) & -0.168 (13) & 0.8897 (4) & 4.86 (1) \\ C(23) & 0.050 (10) & 0.862 (10) & 0.854 (10) & 5.7 (5) & S(12) & 0.0554 (1) & -0.618 (13) & 0.9393 (1) & 4.86 (5) \\ C(24) & 0.060 (10) & 0.865 (10) & 0.954 (10) & 5.7 (5) & S(22) & 1.048 (1) & 0.018 (3) & 0.9393 (1) & 4.86 (5) \\ C(25) & 0.053 (10) & 0.058 (10) & 0.556 (10) & 5.56 (10) & 5.64 (1) & S(13) & 0.3393 (1) & 0.3726 (3) & 0.6383 (2) & 0.353 (1) \\ C(13) & 0.0038 (10) & 0.558 (10) & 0.556 (10) & 5.44 (10) & S(13) & 0.3393 (1) & 0.3726 (3) & 0.6383 (2) & 3.31 (1) \\ C(15) & 0.1038 (10) & 0.558 (10) & 0.4271 (10) & 3.34 (3) & O(11) & 0.2136 (1) & -0.0386 (1) & 0.4383 (2) & 3.01 (1) \\ C(14) & -0.157 (10) & 0.0297 (10) & 0.4471 (10) & 3.34 (3) & O(12) & 0.6868 (2) & -0.0098 (6) & 0.5381 (2) & 3.01 (1) \\ C(15) & 0.1095 (10) & 0.4221 (6) & 0.04971 (10) & 3.34 (6) & O(21) & 0.0488 (1) & 0.318 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.338 (1) & 0.3$	C(12)	0.6061 (10)	0.4797 (8	0.1227 (9)	3.4 (3)	Co(1)	0.78735 (5)	0.0729(1)	0.63754 (4)	2.46 (2)
$ \begin{array}{c} C(14) & 0.796 (10) & 0.3374 (10) & 0.4883 (10) & 61 (3) & Cot3) & 0.4197 (5) & 0.2288 (11) & 0.5897 (4) & 271 (2) \\ C(15) & 0.6790 (10) & 0.334 (7) & 0.3815 (9) & 225 (1) & 51 (1) & 0.7964 (1) & -0.4688 (3) & 0.64997 (8) & 3.34 (5) \\ C(22) & 0.4321 (10) & 0.8295 (10) & 0.5244 (10) & 57 (5) & S(22) & 1.0456 (1) & 0.0181 (3) & 0.8385 (1) \\ C(23) & 0.6321 (10) & 0.8905 (10) & 0.5544 (10) & 57 (5) & S(22) & 1.0456 (1) & 0.0181 (3) & 0.8385 (1) \\ C(24) & 0.6064 (10) & 0.8905 (10) & 0.5544 (10) & 57 (5) & S(22) & 1.0456 (1) & 0.0185 (3) & 0.92733 (9) & 3.64 (5) \\ C(25) & 0.6331 (10) & 0.6373 (0) & 0.7444 (10) & 3.46 (1) & S(31) & 0.4332 (1) & 0.1452 (3) & 0.8335 (3) & 0.3733 (3) & 3.64 (5) \\ C(30) & 0.0331 (10) & 0.0376 (0) & 0.7494 (10) & 3.54 (1) & 2037 (1) & 0.4372 (1) & 0.8337 (2) & 0.8333 (2) & 3.16 (1) \\ C(31) & 0.0338 (10) & 0.4578 (9) & 0.6666 (10) & 4.54 (4) & 2031 & 0.4578 (3) & 0.1737 (6) & 0.8333 (2) & 3.16 (1) \\ C(34) & 0.048 (10) & 0.4498 (9) & 0.6666 (10) & 4.54 (4) & 2031 & 0.4578 (3) & -0.0734 (6) & 0.8373 (2) & 3.16 (1) \\ C(44) & 0.041 (10) & 0.4599 (7) & 0.4044 (10) & 5.34 (4) & 0.031 & 0.4621 (3) & 0.0767 (3) & -0.0734 (6) & 0.8377 (2) & 3.24 (1) \\ C(44) & 0.041 (10) & 0.2587 (9) & 0.4421 (10) & 5.34 (4) & 0.031 & 0.4621 (3) & 0.178 (6) & 0.8377 (2) & 3.24 (1) \\ C(44) & -0.157 (10) & 1.0294 (9) & 0.0314 (10) & 5.34 (4) & 0.031 & 0.4124 (3) & 0.3184 (7) & 0.8496 (2) & 3.31 (1) \\ C(45) & -0.138 (10) & 0.3594 (9) & 0.014 (10) & 5.84 (4) & 0.033 & 0.114 (3) & 0.3184 (7) & 0.8487 (2) & 3.10 (1) \\ C(45) & -0.105 (10) & 0.557 (9) & 0.014 (10) & 5.84 (4) & 0.033 & 0.114 (3) & 0.3184 (7) & 0.3578 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & 0.5378 (1) & $	C(13)	0.6724 (10)	0.4593 (9) 0.0594 (10)	4.9 (4)	Co(2)	1.05291 (5)	-0.1179 (1)	0.88477 (4)	2.98 (2)
C(15) 0.679 (10) 0.4545 (9) 0.121 (10) 3.9 (0) S(12) 0.2775 (3) 0.6797 (3) 1.34 (3) (10) 0.2775 (3) 0.6797 (3) 1.04 (3) 0.7008 (6) 0.7008 (6) 0.555 (1) 0.5753 (10) 0.3622 (9) 0.9797 (10) 4.2 (4) S(12) 0.5554 (1) -0.1681 (3) 0.9503 (1) 4.66 (6) (2) 0.656 (1) 0.556 (1) 0.5753 (10) 0.3622 (9) 0.9797 (10) 4.2 (4) S(22) 1.05554 (1) -0.1681 (3) 0.9503 (1) 0.9503 (10) 0.3555 (1) 0.5753 (10) 0.3755 (10) 0.5753 (10) 0.3755 (10) 0.5753 (10) 0.3750 (10) 3.46 (3) S(21) 0.5753 (1) 0.442 (3) 0.9443 (9) 3.46 (5) C(25) 0.6563 (10) 0.3750 (10) 3.46 (1) 3.46 (1) S(21) 0.3751 (1) 0.442 (3) 0.9443 (9) 3.46 (5) C(25) 0.668 (9) 0.6233 (8) 0.5783 (9) 2.364 (1) 4.53 (1) 0.5373 (1) 0.442 (3) 0.9443 (9) 3.46 (5) C(23) 0.0351 (10) 0.4575 (10) 0.4576 (10) 4.559 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.576 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.276 (10) 4.559 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.764 (10) 2.550 (10) 4.675 (10) 4.675 (10) 4.776 (10) 4.716 (10) 4.526 (10) 4.576 (10) 4.576 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10) 4.577 (10) 4.550 (10	C(14)	0.7066 (10)	0.5374 (1	0) 0.0488 (10)	6.1 (5)	Co(3)	0.41979 (5)	0.2285 (1)	0.86907 (4)	2.71 (2)
$ \begin{array}{c} C(16) & 0.012(19) & 0.0254(1) & 0.010(19) & 32(3) & S(12) & 0.7984(1) & -0.0488(13) & 0.0498(16) & 3.010(19) \\ C(20) & 0.0504(10) & 0.8965(10) & 0.9544(10) & 5.7(5) & S(21) & 1.0486(1) & 0.0185(13) & 0.9886(1) & 0.9876(1) \\ C(20) & 0.0503(10) & 0.8955(10) & 0.9544(10) & 5.7(5) & S(21) & 1.0486(1) & 0.0185(13) & 0.9878(1) & 0.306(1) \\ C(20) & 0.0533(10) & 0.8735(19) & 0.7440(10) & 3.8(4) & S(31) & 0.4332(1) & 0.1422(13) & 0.4943(19) & 3.8(5) \\ C(20) & 0.053(10) & 0.425(16) & 0.057(1) & 0.0442(13) & 0.4943(19) & 3.8(5) \\ C(30) & 0.038(10) & 0.4256(10) & 0.0574(10) & 1.4(4) & S(23) & 0.273(1) & 0.0442(13) & 0.4943(19) & 3.8(5) \\ C(31) & 0.038(10) & 0.4256(19) & 0.0604(19) & 2.2(3) & 0.0173(1) & 0.776(1) & -0.0234(6) & 0.9351(1 & 3.4(10) & 3.8(10) & 0.422(13) & 0.01796(1) & -3.556(1) & 0.9384(1) & 3.4(10) & 5.36(1 & 0.012) & 0.0176(1) & -0.0934(6) & 0.9351(2 & 3.8(1) & 3.4(10) & 3.4(6) & 0.021(1 & 1.030(1) & 0.0422(13) & 0.01796(1) & 3.455(1 & 3.4(10) & 3.4(10) & 0.336(1) & 0.0236(1) & 0.0236(1) & 0.0387(1) & 3.4(10) & 3.4(10) & 0.236(1) & 0.0376(1) & -0.0934(6) & 0.9387(1 & 3.4(1) & 0.4494(10) & 5.36(1 & 0.012) & 0.0136(10) & 0.0376(1) & -0.0234(6) & 0.9387(1 & 3.4(1) & 0.422(1) & 0.0376(1) & -0.0346(1) & 0.338(1) & 0.3184(7) & 0.338(1) & 0.3184(7) & 0.399(1) & 2.7(1) & 0.011(1) & 0.0236(9) & 0.316(100) & 5.36(1 & 0.0237(1) & 0.0331(5) & 0.3384(7) & 0.399(1) & 2.7(1) & 0.011(1) & 0.3285(1) & 0.0387(1) & 0.011(7) & 0.422(2) & 0.011(7) & 0.422(2) & 0.011(7) & 0.422(2) & 0.011(7) & 0.422(2) & 0.011(7) & 0.422(2) & 0.011(7) & 0.422(2) & 0.011(7) & 0.422(2) & 0.011(7) & 0.0235(1) & 0.039(1) & 0.011(7) & 0.0235(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335(1) & 0.0335($	C(15)	0.6796 (10)	0.6345 (9	0.1121(10)	3.9(4)	S(11)	0.8056 (1)	0.2775 (3)	0.67997 (8)	3.24 (5)
$ \begin{array}{c} (22) & 0.233(10) & 0.3822(0) & 0.2797(0) & 4.2(4) & 8(11) & 0.0282(1) & 0.1488(12) & 0.0918(10) & 3.06(15) \\ (22) & 0.2733(10) & 0.2322(0) & 0.2336(10) & 5.5(4) & 8222) & 1.048(1) & 0.0183(1) & 0.9318(10) & 3.61(5) \\ (23) & 0.0383(10) & 0.253(10) & 0.354(10) & 3.5(4) & 8221 & 1.048(1) & 0.0183(1) & 0.9318(10) & 3.61(5) \\ (23) & 0.0183(10) & 0.253(0) & 0.2740(10) & 3.8(4) & 8231 & 0.343(1) & 0.1726(1) & 0.4842(3) & 0.94433(9) & 3.66(5) \\ (23) & 0.0185(10) & 0.4221(8) & 0.0497(10) & 4.1(6) & 8233 & 0.340(1) & 0.1726(1) & 0.4843(2) & 0.48438(1) & 0.376(1) \\ (23) & 0.0195(10) & 0.4221(8) & 0.0497(10) & 3.5(1) & 0.013 & 0.076(1) & -0.008(6) & 0.591(2) & 3.40(1) \\ (24) & 0.0061(10) & 0.459(7) & 0.0604(9) & 2.9(3) & 0.013 & 0.076(1) & -0.008(6) & 0.591(2) & 3.40(1) \\ (24) & 0.0061(10) & 0.459(7) & 0.0604(9) & 2.9(3) & 0.0221 & 1.1330(3) & 0.0422(7) & 0.8486(2) & 3.40(1) \\ (24) & 0.0061(10) & 0.359(7) & 0.0394(10) & 5.3(6) & 0.0221 & 1.1330(3) & 0.0422(7) & 0.8486(2) & 3.40(1) \\ (24) & -0.1576(10) & 1.0284(7) & 0.0378(10) & 4.2(4) & 0.021 & 1.0420(3) & -0.2184(6) & 0.591(2) & 3.40(1) \\ (25) & 0.2374(9) & 0.9669(7) & 0.2178(8) & 2.4(3) & 0.0313(1) & 0.3184(7) & 0.5907(2) & 3.30(1) \\ (25) & 0.2374(9) & 0.9669(7) & 0.2378(10) & 4.7(4) & 0.033 & 0.128(3) & 0.3184(7) & 0.5907(2) & 3.30(1) \\ (25) & 0.4384(10) & 0.3284(9) & 0.0374(10) & 4.0(3) & N(12) & 0.5776(3) & -0.0281(7) & 0.5907(3) & 3.30(1) \\ (25) & 0.4384(10) & 0.3284(9) & 0.0370(10) & 4.0(3) & N(12) & 0.5776(3) & -0.0281(7) & 0.5977(3) & 3.00(1) \\ (25) & 0.4384(10) & 0.3284(9) & 0.0371(10) & 4.0(3) & N(12) & 0.5776(3) & -0.0281(7) & 0.5977(3) & 3.00(1) \\ (25) & 0.4384(10) & 0.5384(10) & 0.550(10) & N(12) & 0.5776(3) & -0.0281(7) & 0.5377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) & 0.3377(3) $	C(16)	0.6121 (9)	0.6534 (8	0.1810(9)	3.0 (3) 2.5 (3)	S(12)	0.7584 (1)	-0.0458 (3)	0.70088 (8)	3.10(5)
$ \begin{array}{c} 2129 \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\ (225) \\$	C(22)	0.4200 (9)	0.8334 (7	0.0013(9)	$\frac{2.3(3)}{42(4)}$	S(13)	0.6926(1)	0.1468 (3)	0.01818(9)	3.34 (3)
$ \begin{array}{c} cross \\ cross $	C(23)	0.5525 (10)	0.8022 (9	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $	5.7 (5)	S(21) S(22)	0.9554(1)	-0.1081(3)	0.8850(1)	3.61 (5)
$ \begin{array}{c} \hline class 1 (0) & 0.873 (0) & 0.740 (10) & 38 (4) & sc(1) & 0.442 (1) & 0.442 (3) & 0.8433 (9) & 3.36 (5) \\ \hline class 0 & 0.018 (10) & 0.558 (9) & 0.7190 (10) & 41 (4) & sc(3) & 0.3570 (1) & 0.0442 (3) & 0.8433 (9) & 3.36 (5) \\ \hline class 0 & 0.018 (10) & 0.558 (9) & 0.661 (10) & 4.36 (0) & 0.13 (0) & 0.5776 (3) & -0.0984 (6) & 0.8833 (5) & 3.70 (5) \\ \hline class 0 & 0.055 (10) & 0.422 (18) & 0.6847 (10) & 3.3 (3) & 0.(12) & 0.8689 (2) & -0.0984 (6) & 0.8833 (2) & 3.1 (1) \\ \hline class 0 & 0.068 (10) & 0.482 (10) & 0.482 (10) & 3.3 (3) & 0.(12) & 0.8689 (2) & -0.0984 (6) & 0.847 (2) & 3.4 (1) \\ \hline class 0 & 0.068 (10) & 0.482 (10) & 0.489 (10) & 3.2 (4) & 0.013 (10) & 0.0576 (3) & -0.0984 (6) & 0.847 (2) & 3.4 (1) \\ \hline class 0 & 0.068 (10) & 0.930 (9) & 0.0189 (10) & 3.2 (4) & 0.023 (1) & 0.0058 (1) & 0.8485 (2) & 3.3 (1) \\ \hline class 0 & -0.083 (10) & 0.939 (9) & 0.0494 (10) & 5.8 (4) & 0.023 (1) & 0.060 (3) & -0.314 (7) & 0.8845 (2) & 3.3 (1) \\ \hline class 0 & -0.183 (10) & 0.0396 (9) & 0.4043 (10) & 5.8 (4) & 0.023 (1) & 0.4833 (3) & 0.3184 (7) & 0.807 (2) & 3.1 (1) \\ \hline class 0 & 0.3274 (9) & 0.0908 (9) & 0.3176 (8) & 2.4 (3) & 0.013 (0) & 4.833 (3) & 0.3184 (7) & 0.807 (2) & 3.1 (1) \\ \hline class 0 & 0.102 (8) & 0.316 (10) & 3.6 (3) & N(11) & 0.833 (3) & 0.3184 (7) & 0.807 (2) & 3.1 (2) \\ \hline class 0 & 0.102 (8) & 0.2867 (10) & 4.0 (3) & N(12) & 0.873 (3) & 0.3184 (7) & 0.801 (2) & 2.4 (1) \\ \hline class 0 & 0.102 (8) & 0.2867 (10) & 4.0 (3) & N(12) & 0.873 (3) & 0.3184 (7) & 0.801 (2) & 2.4 (1) \\ \hline class 0 & 0.0234 (10) & 0.5384 (10) & 0.558 (10) & 4.0 (3) & N(12) & 0.833 (3) & 0.0176 (6) & 0.401 (2) & 2.4 (1) \\ \hline class 0 & 0.0234 (1) & 0.6278 (8) & 0.2967 (10) & 0.1384 (1) & 0.581 (1) & 0.668 (1) & 0.707 (1) & 2.4 (2) \\ \hline class 0 & 0.0234 (1) & 0.6278 (1) & 0.558 (10) & 4.0 (2) & 1.000 (2) & 0.0034 (9) & 0.218 (7) & 0.831 (1) & 0.558 (1) & 0.608 (1) & 0.707 (1) & 2.4 (2) \\ \hline class 0 & 0.0234 (1) & 0.558 (10) & 0.578 (1) & 0.058 (1) & 0.058 (1) & 0.578 (1) & 0.578 (1) & 0.578 (1) & 0.578 (1) & 0.578 (1) & 0.578 (1) & 0.578 (1) & 0.5$	C(24)	0.5733 (10)	0.9038 (1	0) 0.8361 (10)	5.6 (4)	S(22) S(23)	1.0758 (1)	-0.3205(3)	0.92733(9)	4.40 (6)
$ \begin{array}{c} \hline (212) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213) \\ (213$	C(26)	0.4633 (10)	0.8735 (9	0.7440 (10)	3.8 (4)	S(31)	0.4332 (1)	0.1482 (3)	0.94483 (9)	3.80 (5)
$ \begin{array}{c} C(33) & 0.0138 (10) & 0.558 (e) & 0.7199 (10) & 4.1 (4) & S(33) & 0.3430 (1) & 0.3726 (3) & 0.88856 (8) & 3.70 (5) \\ C(35) & 0.1095 (10) & 0.4221 (8) & 0.6647 (10) & 3.5 (3) & 0.(12) & 0.8698 (2) & -0.00934 (6) & 0.6537 (2) & 3.2 (1) \\ C(36) & 0.164 (10) & 0.4859 (7) & 0.6049 (9) & 2.3 (3) & 0.776 (3) & 0.6438 (10) & 0.421 (4) & 0.0211 & 10.963 (3) & 0.04934 (6) & 0.5874 (2) & 3.4 (1) \\ C(42) & 0.0691 (9) & 0.0439 (9) & 0.6049 (9) & 2.4 (4) & 0.211 & 10.963 (3) & 0.04934 (6) & 0.5877 (2) & 3.4 (1) \\ C(44) & -0.157 (10) & 1.1025 (9) & 0.4043 (10) & 5.8 (4) & 0.211 & 10.963 (3) & 0.0424 (7) & 0.8845 (2) & 3.7 (1) \\ C(45) & -0.1331 (10) & 0.9395 (9) & 0.4043 (10) & 5.8 (4) & 0.211 & 0.0423 (3) & 0.1078 (6) & 0.8877 (2) & 3.1 (1) \\ C(52) & 0.3274 (9) & 0.9069 (7) & 0.3178 (8) & 2.4 (3) & 0.033 & 0.4124 (3) & 0.3184 (7) & 0.5901 (2) & 2.7 (1) \\ C(54) & 0.1829 (10) & 1.0125 (8) & 0.267 (10) & 4.0 (3) & N(12) & 0.8752 (2) & -0.1034 (8) & 0.8397 (2) & 3.3 (1) \\ C(55) & 0.4214 (10) & 0.6129 (8) & 0.3580 (10) & 5.6 (4) & N(22) & 0.1996 (3) & 0.0128 (6) & 0.8377 (2) & 3.6 (2) \\ C(56) & 0.4631 (10) & 0.651 (10) & 5.761 (0) & 7.1 (5) & N(31) & 0.3764 (7) & 0.9218 (3) & 3.7 (2) \\ C(56) & 0.4631 (10) & 0.5781 (10) & 0.7067 (1) & -0.1234 (8) & 0.5897 (3) & 3.7 (2) \\ C(56) & 0.4631 (10) & 0.5931 (10) & 0.7167 (10) & 7.1 (5) & N(31) & 0.3161 (3) & 0.3374 (7) & 9.3031 (3) & 3.3 (2) \\ C(66) & 0.5965 (10) & 0.6572 (8) & 0.5734 (9) & 3.7 (2) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.5734 (9) & 3.7 (2) \\ C(11) & 0.8323 (4) & 0.3531 (9) & 0.6326 (3) & 2.4 (2) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.5744 (9) & 3.7 (2) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.5581 (4) & 4.9 (3) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.558 (4) & 4.9 (3) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.558 (4) & 4.9 (3) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.558 (4) & 4.9 (3) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.558 (4) & 4.9 (3) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.558 (4) & 4.9 (3) \\ C(11) & 0.8323 (4) & 0.3531 (10) & 0.558 (4) & 4.9 (2) \\ C(11) & 0.8323 (4) $	C(32)	0.0689 (9)	0.6233 (8	6) 0.7083 (9)	2.8 (3)	S(32)	0.3570(1)	0.0442 (3)	0.84933 (9)	3.65 (5)
$\begin{array}{c} C(34) & 0.0338 (10) & 0.4578 (9) & 0.6664 (10) & 4.5 (4) & 0.(11) & 0.8219 (3) & 0.1739 (3) & 0.6583 (2) & 3.1 (1) \\ C(35) & 0.105 (10) & 0.4523 (2) & 0.6004 (9) & 23 (3) & 0.(73) & 0.767 (3) & -0.0098 (6) & 0.557 (2) & 3.2 (1) \\ C(42) & 0.001 (9) & 0.949 (8) & 0.558 (9) & 2.4 (3) & 0.(23) & 1.1030 (3) & 0.0452 (7) & 0.866 (2) & 3.5 (1) \\ C(44) & -0.1157 (10) & 1.10394 (9) & 0.5034 (10) & 5.3 (4) & 0.021 & 1.1360 (3) & 0.0745 (6) & 0.8877 (2) & 3.1 (1) \\ C(45) & -0.1151 (10) & 0.8557 (9) & 0.4215 (10) & 4.7 (4) & 0.022 & 0.4856 (3) & 0.0734 (6) & 0.8877 (2) & 3.1 (1) \\ C(54) & -1.015 (10) & 0.8557 (9) & 0.4215 (10) & 4.7 (4) & 0.021 & 0.4823 (3) & 0.0186 (6) & 0.807 (2) & 3.3 (1) \\ C(52) & 0.3271 (9) & 0.906 (7) & 0.3178 (8) & 2.4 (3) & 0.033 & 0.4124 (3) & 0.3108 (6) & 0.8071 (2) & 3.0 (1) \\ C(55) & 0.129 (10) & 1.0125 (8) & 0.207 (10) & 4.0 (3) & N1(1) & 0.8331 (3) & 0.0184 (6) & 0.8071 (2) & 3.0 (1) \\ C(55) & 0.1329 (10) & 0.1025 (8) & 0.037 (10) & 4.0 (3) & N1(1) & 0.8373 (3) & 0.0172 (18) & 0.8372 (3) & 3.1 (2) \\ C(56) & 0.189 (10) & 0.3288 (9) & 0.104 (10) & 4.5 (4) & N1(3) & 0.7076 (3) & -0.1051 (7) & 0.6917 (2) & 2.6 (1) \\ C(56) & 0.6802 (10) & 0.5738 (10) & 0.5790 (10) & 4.4 (4) & N1(2) & 0.9705 (3) & 0.00271 (8) & 0.8372 (3) & 3.3 (2) \\ C(16) & 0.6602 (10) & 0.5738 (10) & 0.5790 (10) & 4.4 (4) & N1(2) & 0.9705 (3) & 0.0371 (8) & 0.3872 (3) & 3.2 (2) \\ C(10) & -661 & 0.5738 (10) & 0.573 (4) & 3.37 (3) & N230 (3) (30 (10) & 0.3877 (8) & 0.5794 (4) & 2.2 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.33 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.33 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.33 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6374 (4) & 3.3 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.4 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.4 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.4 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6326 (4) & 2.4 (2) \\ C(11) & 0.8253 (4) & 0.3378 (10) & 0.6354 (4) & 3.3 (2) \\ C(11) & 0.8253 (4) & 0$	C(33)	0.0138 (10)	0.5586 (9) 0.7190 (10)	4.1 (4)	S(33)	0.3430(1)	0.3726 (3)	0.88365 (8)	3.70 (5)
$\begin{array}{c} C(35) & 0.1095 (10) & 0.4221 (8) & 0.6491 (10) & -35.13 & 0.0(12) & 0.8698 (2) & -0.00934 (6) & 0.5537 (2) & 3.2 (1) \\ C(42) & 0.0041 (9) & 0.9469 (8) & 0.6358 (9) & 24.31 & 0.0211 & 1.0303 (3) & 0.0432 (7) & 0.8466 (2) & 3.6 (1) \\ C(42) & -0.0571 (10) & 1.0394 (9) & 0.5313 (10) & 2.43 & 0.0211 & 1.1382 (1) & -0.2354 (7) & 0.8466 (2) & 3.7 (1) \\ C(45) & -0.1571 (9) & 1.0057 (9) & 0.4031 (10) & 5.8 (4) & 0.0311 & 0.4232 (3) & 0.0376 (6) & 0.8877 (2) & 3.1 (1) \\ C(45) & -0.1571 (9) & 1.0025 (8) & 0.3161 (10) & 3.6 (4) & 0.0311 & 0.4323 (3) & 0.1078 (6) & 0.8877 (2) & 3.3 (1) \\ C(52) & 0.3274 (9) & 0.9069 (7) & 0.3178 (8) & 2.4 (3) & 0.0133 & 0.4124 (3) & 0.3184 (7) & 0.5901 (2) & 2.7 (1) \\ C(54) & 0.1829 (10) & 1.0125 (8) & 0.2067 (10) & 4.0 (3) & N(12) & 0.8753 (3) & -0.1234 (8) & 0.8874 (2) & 3.5 (2) \\ C(55) & 0.1490 (10) & 0.9280 (9) & 0.1014 (10) & 4.5 (4) & N(13) & 0.8753 (3) & -0.1234 (8) & 0.8374 (3) & 3.5 (2) \\ C(55) & 0.1498 (10) & 0.8388 (9) & 0.0055 (9) & 3.7 (4) & N(21) & 0.9705 (3) & 0.0721 (8) & 0.3371 (3) & 3.3 (2) \\ C(64) & 0.6611 (10) & 0.5554 (10) & 0.6671 (10) & 7.1 (6) & N(12) & 0.9705 (3) & 0.0234 (9) & 0.921 (8) & 3.3 (7) \\ C(66) & 0.6620 (10) & 0.5737 (10) & 0.771 (0) & 7.1 (6) & N(12) & 0.301 (7) & 0.3512 (1) & 2.4 (1) \\ C(11) & 0.8323 (4) & 0.3512 (10) & 0.5794 (4) & 3.7 (2) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.8271 (4) & -0.3551 (6) & 4.7 (8) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.8371 (6) & 0.3551 (6) & 4.7 (8) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.8373 (4) & 0.3931 (10) & 0.5750 (4) & 3.2 (2) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.8373 (4) & 0.3931 (6) & 0.5550 (4) & 4.7 (8) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.8373 (6) & 0.3551 (6) & 4.7 (8) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.8373 (5) & 0.3751 (6) & 0.3551 (6) & 4.7 (8) \\ C(11) - S(1) & 2.200 (4) & C(2) - S(3) & 2.208 (3) & C(11) & 0.3751 (6) & 0.3551 (6) & 4.7 (6) $	C(34)	0.0338 (10)	0.4578 (9	0) 0.6664 (10)	4.5 (4)	O(11)	0.8219 (3)	0.1739 (6)	0.5832 (2)	3.1 (1)
$ \begin{array}{c} C_{130} & 0.166 (10) & 0.439 (f) & 0.004+ (f) & 24 (f) & 0.013 & 0.76^{+} (f) & -0.0432 (f) & 0.544 (f) & 0.542 (f) & 0.5454 (f) & 0.542 (f) & 0.5454 (f) & 0.545 (f) & 0.5454 (f) & 0.5454 (f) & 0.5454 (f) & 0.555 (f) & 0.744 (f) & 0.5454 (f) & 0.5554 (f) &$	C(35)	0.1095 (10)	0.4221 (8	3) 0.6047 (10)	3.5 (3)	O(12)	0.8689 (2)	-0.0098 (6)	0.6537 (2)	3.2 (1)
$ \begin{array}{c} 142, & 0.00691 (9), & 0.0489 (10), & 0.0489 (10), & 42 (4), & 0.(41), & 1.0383 (1), & 0.0484 (1), & 0.888 (1), & 0.888 (1), & 0.888 (1), & 0.1018 (10), & 0.888 (1), & 0.1018 (10), & 0.887 (2), & 3.1 (1), & 0.1018 (10), & 0.887 (2), & 3.1 (1), & 0.1018 (10), & 0.887 (2), & 3.1 (1), & 0.1018 (10), & 0.887 (2), & 3.1 (1), & 0.1018 (10), & 0.887 (2), & 3.1 (1), & 0.1018 (10), & 0.887 (2), & 3.1 (1), & 0.1018 (10), & 0.1018 (10), & 0.1018 (10), & 0.1018 (10), & 0.831 (1), & 0.313 (13), & 0.1124 (1), & 0.313 (13), & 0.3184 (7), & 0.5901 (2), & 2.7 (1), & 0.10218 (1), & 0.1025 (10), & 4.7 (4), & 0.1018 (1), & 0.833 (1), & 0.3184 (7), & 0.5901 (2), & 2.7 (1), & 0.1018 (10), & 0.025 (10), & 4.0 (3), & 0.112 (1), & 0.833 (1), & 0.3184 (7), & 0.5901 (2), & 2.7 (1), & 0.1011 (10), & 0.258 (0), & 0.1025 (10), & 0.1025 (10), & 0.1025 (10), & 0.1025 (10), & 0.1025 (10), & 0.1028 (10), & 0.0326 (1), & 0.0334 (10), & 0.331 (13), & 3.1 (2), & 0.1018 (10), & 0.3888 (0), & 0.0055 (0), & 3.7 (4), & N(12), & 0.9705 (3), & 0.0214 (10), & 0.4381 (10), & 0.355 (10), & 0.6574 (10), & 5.84 (4), & N(21), & 0.9705 (3), & 0.0214 (10), & 0.3331 (13), & 3.1 (2), & 0.1618 (1), & 0.3331 (1), & 0.3124 (1), & 0.3331 (1), & 0.3331 (1), & 3.1 (2), & 0.1618 (1), & 0.3331 (1), & 0.3331 (1), & 3.1 (2), & 0.1618 (1), & 0.3331 (1), & 0.3331 (1), & 3.1 (2), & 0.1618 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & 0.3331 (1), & $	C(36)	0.1661 (10)	0.4859 (/	0.6004(9)	2.9(3)	O(13)	0.7676 (3)	-0.0934 (6)	0.5941 (2)	3.4 (1)
$ \begin{array}{c} c_{143}^{$	C(42)	0.0041(9)	0.9409 (8	0.0302(9)	2.8 (5) 4 2 (4)	0(21)	1.0303 (3)	0.0432 (7)	0.8400 (2)	3.0(1) 3.9(1)
$\begin{array}{cccccc} -0.1831 (10) & 0.396 (e) & 0.403 (10) & 58 (e) & 0.31 & 0.4221 (3) & 0.178 (e) & 0.8495 (72) & 31 (1) \\ (C46) & -0.105 (10) & 0.857 (9) & 0.4215 (10) & 4.74 (4) & 0.33 & 0.4124 (3) & 0.3184 (7) & 0.8495 (2) & 3.3 (1) \\ (C3) & 0.271 (9) & 1.0025 (8) & 0.306 (10) & 4.03 (3) & 0.110 & 8(6) & 0.3077 (2) & 3.0 (1) \\ (C4) & 0.1829 (10) & 1.0125 (8) & 0.2067 (10) & 4.0 (3) & N(12) & 0.8752 (3) & -0.110 (7) & 0.6917 (2) & 2.6 (1) \\ (C5) & 0.1401 (10) & 0.2920 (9) & 0.1014 (10) & 4.54 (4) & N(13) & 0.0766 (3) & 0.3384 (7) & 0.8986 (2) & 0.3782 (3) & 0.3184 (7) & 0.8987 (3) & 0.3287 (3) & 0.3287 (3) & 0.3287 (3) & 0.3287 (3) & 0.3287 (3) & 0.3287 (3) & 0.3287 (3) & 0.3287 (3) & 0.3281 (3) & 3.3 (2) \\ (C6) & 0.4838 (10) & 0.5854 (10) & 0.6610 (10) & 5.8 (4) & N(22) & 1.1596 (3) & 0.3297 (7) & 0.4277 (3) & 3.0 (2) \\ (C4) & 0.6620 (10) & 0.6378 (10) & 0.6790 (10) & 6.4 (5) & N(32) & 0.4716 (3) & -0.3378 (8) & 0.3338 (8) & 0.3536 (3) & 2.28 (1) \\ (C46) & 0.6620 (10) & 0.6378 (10) & 0.6790 (10) & 6.4 (5) & N(32) & 0.4716 (3) & -0.3378 (10) & 0.5394 (4) & 3.0 (2) \\ (C11) & 0.8225 (4) & 0.3573 (4) & 0.3576 (1) & 0.5396 (4) & 0.7378 (4) & 0.3536 (3) & 2.28 (1) \\ (C11) & 0.8225 (4) & 0.3578 (4) & 0.3578 (1) & 0.5396 (4) & 7.0325 (2) & 2.0 (2) \\ (C11) & 0.8225 (4) & 0.5378 (10) & 0.5596 (4) & 4.3 (3) \\ (C11) & 0.8526 (4) & 0.3738 (10) & 0.5596 (4) & 4.3 (3) \\ (C11) & 0.8526 (4) & 0.3738 (10) & 0.5596 (4) & 4.3 (3) \\ (C11) & 0.5591 (4) & 0.5596 (4) & 2.213 (3) & C(2) & 0.277 (4) & 0.3573 (1) & 0.5558 (4) & 3.24 (2) \\ (C11) & 0.8526 (4) & 0.3738 (10) & 0.5596 (4) & 4.3 (3) & 2.20 (4) \\ (C12) & 0.8526 (4) & 0.3738 (10) & 0.5596 (4) & 4.3 (3) & 2.20 (2) \\ (C11) & 0.8516 (4) & 0.3578 (1) & 0.5558 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.5578 (1) & 0.$	C(43) C(44)	-0.1576(10)	1.0294 (9	0.5034(10)	5.3 (4)	O(22)	1.1382 (3)	-0.2314(7)	0.8266 (2)	3.7(1)
$ \begin{array}{c} \hline C(4) \\ C(3) \\$	C(45)	-0.1831(10)	0.9396 (9) 0.4043 (10)	5.8 (4)	O(31)	0.4823 (3)	0.3745 (6)	0.8877 (2)	3.1(1)
$ \begin{array}{c} C(52) \\ C(53) \\ C(54) \\ C(54) \\ C(54) \\ C(54) \\ C(54) \\ C(55) \\ C(54) \\ C(54) \\ C(55) \\ C(56) \\ C(56) \\ C(56) \\ C(52) \\ C(56) \\ C(56) \\ C(57) \\ C(56) \\ C(57) \\ C(56) \\ C(57) $	C(46)	-0.1105 (10)	0.8557 (9	0.4215 (10)	4.7 (4)	O(32)	0.4850 (3)	0.1078 (6)	0.8495 (2)	3.3 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(52)	0.3274 (9)	0.9069 (7	7) 0.3178 (8)	2.4 (3)	O(33)	0.4124 (3)	0.3108 (6)	0.8037 (2)	3.0 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(53)	0.2771 (9)	1.0025 (8	3) 0.3161 (10)	3.6 (3)	N(11)	0.8331 (3)	0.3184 (7)	0.5901 (2)	2.7 (1)
$\begin{array}{cccccc} C(55) & 0.1401 (10) & 0.9280 (9) & 0.1014 (10) & 4-3 (4) & N(13) & 0.7076 (3) & -0.1204 (8) & 0.8346 (2) & 1.5 (2) \\ C(56) & 0.4824 (10) & 0.6129 (8) & 0.5580 (10) & 4.0 (3) & N(22) & 1.1596 (3) & 0.0721 (8) & 0.8327 (3) & 3.3 (2) \\ C(61) & 0.4824 (10) & 0.5284 (10) & 0.0610 (10) & 5.4 (4) & N(22) & 1.1596 (3) & 0.0724 (8) & 0.8324 (3) & 3.3 (2) \\ C(64) & 0.4831 (10) & 0.5931 (10) & 0.7167 (10) & 7.1 (5) & N(31) & 0.5124 (3) & -0.3397 (8) & 0.8331 (3) & 3.3 (2) \\ C(66) & 0.5602 (10) & 0.6672 (8) & 0.5734 (9) & 3.7 (3) & N(32) & 0.4716 (3) & -0.0359 (7) & 0.8427 (3) & 3.3 (2) \\ C(66) & 0.5965 (10) & 0.6672 (8) & 0.5734 (9) & 3.7 (3) & N(33) & 0.610 (3) & 0.3877 (8) & 0.7944 (2) & 2.9 (2) \\ C(111) & 0.8225 (4) & 0.3877 (8) & 0.7944 (2) & 2.9 (2) \\ C(112) & 0.8325 (5) & 0.6119 (10) & 0.5596 (4) & 4.3 (8) \\ C(114) & 0.8433 (5) & 0.5737 (10) & 0.5596 (4) & 4.3 (8) \\ C(114) & 0.8433 (5) & 0.5737 (10) & 0.5596 (4) & 4.3 (8) \\ C(114) & 0.8433 (5) & 0.5737 (10) & 0.5596 (4) & 4.3 (8) \\ C(115) & 0.8359 (4) & 0.3957 (10) & 0.5596 (4) & 4.3 (8) \\ C(1) - S(5) & 2.199 (3) & Co(2) - S(3) & 2.2016 (4) & C1121 & 0.3826 (4) & -0.2376 (10) & 0.5591 (3) & 3.3 (2) \\ C(0)S(6) & 2.208 (3) & Co(2) - S(4) & 2.213 (3) & C1120 & 0.388 (4) & -0.2357 (10) & 0.5590 (4) & 4.3 (2) \\ C(0)O(5) & 1.943 (8) & Co(2) - O(2) & 1.942 (7) & C1120 & 0.3928 (4) & -0.2056 (10) & 0.591 (3) & 3.3 (2) \\ C(0)O(5) & 1.943 (8) & Co(2) - O(2) & 1.942 (7) & C1130 & 0.6956 (4) & -0.095 (10) & 0.5979 (4) & 6.0 (3) \\ S(5) - CC20 & 1.73 (2) & S(3) - C(2) & 1.72 (2) & C1130 & 0.6956 (4) & -0.095 (10) & 0.5979 (4) & 6.0 (3) \\ S(5) - CC30 & 1.70 (1) & S(4) - C(42) & 1.73 (2) & C1130 & 0.6956 (4) & -0.056 (10) & 0.5979 (4) & 6.0 (3) \\ S(5) - CC66 & 1.70 (1) & S(4) - C(2) & 1.72 (2) & C1130 & 0.6956 (4) & -0.0571 (10) & 0.5699 (4) & 6.0 (3) \\ S(5) - CC66 & 1.70 (1) & S(4) - C(2) - C(3) & 1.021 (2) & 0.5975 (5) & -0.1337 (10) & 0.5699 (4) & 6.0 (3) \\ O(1) - N(1) & 1.34 (2) & O(2) - N(1) & 1.33 (2) & C(1130 & 0.6956 (5) & -0.3373 (10) & 0.5999 (4) &$	C(54)	0.1829 (10)	1.0125 (8	B) 0.2067 (10)	4.0 (3)	N(12)	0.8752 (3)	-0.1051 (7)	0.6917 (2)	2.6(1)
$ \begin{array}{c} C(56) & 0.1896 (10) & 0.8388 (9) & 0.103 (9) & 2.1(9) & N(21) & 0.9/16 (5) & 0.0024 (8) & 0.827 (5) & 3.5 (2) \\ C(62) & 0.4284 (10) & 0.66129 (8) & 0.5580 (10) & 0.5580 (10) & 1.56 (3) & 0.0374 (8) & 0.2371 (8) & 0.3331 (3) & 3.3 (2) \\ C(65) & 0.6620 (10) & 0.6378 (10) & 0.6610 (10) & 5.8 (4) & N(22) & 1.156 (3) & 0.0359 (7) & 0.8427 (3) & 3.0 (2) \\ C(65) & 0.6620 (10) & 0.6378 (10) & 0.6790 (10) & 6.4 (5) & N(32) & 0.4716 (3) & -0.0339 (7) & 0.8427 (3) & 3.0 (2) \\ C(66) & 0.5965 (10) & 0.6672 (8) & 0.5734 (9) & 3.7 (3) & N(33) & 0.3610 (3) & 0.3877 (8) & 0.7904 (2) & 2.9 (2) \\ C(111) & 0.8235 (4) & 0.3831 (9) & 0.6526 (3) & 2.16 (2) \\ C(112) & 0.8235 (4) & 0.3831 (9) & 0.6526 (3) & 2.26 (2) \\ C(113) & 0.8325 (5) & 0.5373 (10) & 0.5550 (4) & 4.9 (3) \\ C(11-S(1) & 2.200 (4) & Co(2)-8(3) & 2.208 (3) & C(112) & 0.8379 (4) & 0.3904 (10) & 0.5521 (3) & 4.2 (2) \\ C(11-S(5) & 2.199 (3) & Co(2)-8(3) & 2.208 (3) & C(122) & 0.8368 (4) & -0.305 (10) & 0.7560 (3) & 3.9 (2) \\ Co(1)-S(5) & 2.299 (3) & Co(2)-8(3) & 2.201 (4) & C(122) & 0.8368 (4) & -0.305 (10) & 0.7660 (3) & 3.9 (2) \\ Co(1)-S(6) & 2.203 (3) & Co(2)-8(3) & 2.213 (3) & C(124) & 0.9399 (4) & -0.624 (10) & 0.7590 (3) & 3.1 (2) \\ Co(1)-O(5) & 1.945 (8) & Co(2)-O(3) & 1.932 (7) & C(133) & 0.6638 (4) & -0.0502 (10) & 0.5791 (3) & 3.4 (2) \\ Co(1)-O(6) & 1.945 (8) & Co(2)-O(3) & 1.932 (7) & C(133) & 0.6638 (4) & -0.0502 (10) & 0.5918 (3) & 3.3 (2) \\ Co(1)-O(6) & 1.945 (8) & Co(2)-O(3) & 1.932 (7) & C(133) & 0.6632 (5) & -0.182 (10) & 0.5901 (4) & 6.3 (3) \\ C(1)-O(1) & 1.34 (2) & CO(2)-O(2) & 1.72 (2) & 0.6672 (5) & -0.182 (10) & 0.5901 (4) & 6.3 (3) \\ C(1)-O(1) & 1.34 (2) & CO(2)-O(2) & 1.72 (2) & 0.6672 (5) & -0.182 (10) & 0.5901 (4) & 6.3 (3) \\ C(1)-O(1) & 1.34 (2) & CO(2)-O(2) & 1.124 (1) & C(133) & 0.6632 (5) & -0.182 (10) & 0.5801 (4) & 6.3 (3) \\ C(1)-O(1) & 1.34 (2) & CO(2)-O(2) & 1.124 (2) & 0.0630 (5) & 0.136 (10) & 0.8198 (4) & 6.3 (3) \\ C(1)-O(1) & 1.34 (2) & CO(2)-O(2) & 810 (2) & 2.110 (2) & 0.0780 (1) & 0.9921 (3) & 3.5 (2) \\ C(1)-O(1) & 1.34 (2) $	C(55)	0.1401 (10)	0.9280 (9	9) 0.1014 (10)	4.5 (4)	N(13)	0.7076 (3)	-0.1204 (8)	0.5846 (2)	3.5 (2)
$ \begin{array}{c} C(b) \\ C(b) \\ C(c) \\ C$	C(56)	0.1898 (10)	0.8388 (9	(9) 0.1055(9) 0.5580(10)	3.7 (4) 4.0 (3)	N(21)	0.9705 (3)	0.0/21(8)	0.8327(3)	3.3(2) 3.7(2)
$ \begin{array}{c} C(6) & 0.6351 (10) & 0.2331 (10) & 0.7167 (10) & 71 (5) \\ C(66) & 0.6620 (10) & 0.6378 (10) & 0.5794 (10) & 4.459 \\ C(66) & 0.6620 (10) & 0.6378 (10) & 0.5794 (10) & 4.459 \\ C(66) & 0.5965 (10) & 0.6672 (8) & 0.5734 (9) & 3.7 (3) \\ C(11) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.9 (2) \\ C(111) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.9 (2) \\ C(112) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.4 (2) \\ C(113) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.4 (2) \\ C(113) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.4 (2) \\ C(113) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.4 (2) \\ C(113) & 0.8235 (4) & 0.3877 (8) & 0.7994 (2) & 2.4 (2) \\ C(113) & 0.8235 (4) & 0.3571 (10) & 0.5596 (4) & 4.7 (8) \\ C(114) & 0.0864 (5) & 0.3571 (10) & 0.5596 (4) & 4.7 (8) \\ C(115) & 0.839 (4) & 0.3994 (10) & 0.5551 (3) & 4.2 (2) \\ C(11-5(5) & 2.199 (3) & Co(2)-S(3) & 2.201 (4) \\ C(122) & 0.8368 (4) & -0.2376 (10) & 0.7550 (3) & 3.2 (2) \\ C(1)S(5) & 2.199 (3) & Co(2)-S(3) & 2.201 (4) \\ C(122) & 0.8368 (4) & -0.030 (10) & 0.7666 (3) & 3.9 (2) \\ C(1)O(5) & 1.943 (7) & Co(2)-O(3) & 1.932 (7) \\ C(130) & 0.6936 (4) & -0.0561 (0) & 0.702 (3) & 3.3 (2) \\ C(1)O(5) & 1.943 (7) & Co(2)-O(3) & 1.932 (7) \\ C(130) & 0.6936 (4) & -0.046 (10) & 0.5918 (3) & 3.3 (2) \\ C(1)O(5) & 1.943 (7) & Co(2)-O(3) & 1.932 (7) \\ C(130) & 0.6936 (4) & -0.0567 (10) & 0.580 (4) & 6.6 (3) \\ S(5)-C(52) & 1.73 (2) & S(3)-C(2) & 1.72 (2) & C(133) & 0.6936 (4) & -0.0567 (10) & 0.580 (4) & 6.6 (3) \\ S(5)-C(52) & 1.73 (2) & S(3)-C(2) & 1.72 (2) & C(133) & 0.6935 (5) & -0.2837 (10) & 0.5560 (4) & 4.5 (2) \\ C(1)O(1) & 1.34 (2) & O(2)N(3) & 1.33 (2) & C(211) & 0.9280 (4) & -0.077 (10) & 0.899 (3) & 3.5 (2) \\ C(5)N(51) & 1.38 (2) & O(3)N(31) & 1.33 (2) & C(211) & 0.9280 (4) & -0.077 (10) & 0.899 (3) & 3.5 (2) \\ C(5)N(51) & 1.38 (2) & O(3)N(31) & 1.33 (2) & C(211) & 0.9280 (4) & -0.077 (10) & 0.899 (3) & 3.5 (2) \\ C(5)N(51) & 1.38 (2) & O(3)N(31) & 1.33 (2) & C(211) & 0.9280 (4) & -0.077 (10) & 0.899 (3) & 3.5 (2) \\ C(6)N(61) & 1.36 (1) & O(0N-O(4) &$	C(62)	0.4234 (10)	0.0129 (0	0.5580(10)	5 8 (4)	N(22)	1.1390 (3)	0.0304 (9)	0.9218(3) 0.8331(3)	3.7(2) 3.3(2)
$ \begin{array}{c} C(65) & 0.6620 (10) & 0.6378 (10) & 0.6790 (10) & 6.4 (5) & V(22) & 4.71 (61) & -0.0359 (7) & 0.8427 (23) & 3.0 (21) \\ C(66) & 0.5965 (10) & 0.6672 (8) & 0.5734 (9) & 3.7 (3) & V(33) & 0.3610 (3) & -0.3877 (8) & 0.67904 (2) 2.9 (2) \\ C(112) & 0.8323 (44) & 0.5377 (8) & 0.6354 (4) & 3.9 (2) \\ C(112) & 0.8323 (44) & 0.5377 (10) & 0.6354 (4) & 3.9 (2) \\ C(112) & 0.8323 (44) & 0.5375 (10) & 0.6354 (4) & 4.9 (3) \\ C(114) & 0.8434 (3) & 0.5375 (10) & 0.5550 (4) & 4.2 (3) \\ C(11-8(1)) & 2.200 (4) & Co(2)-S(2) & 2.206 (3) & C(121) & 0.8273 (4) & -0.1356 (9) & 0.7170 (3) & 2.4 (2) \\ Co(1)-S(1) & 2.190 (3) & Co(2)-S(3) & 2.201 (4) & C(122) & 0.8286 (4) & -0.2376 (10) & 0.7550 (3) & 3.2 (2) \\ Co(1)-S(6) & 2.208 (3) & Co(2)-S(3) & 2.201 (4) & C(124) & 0.8286 (4) & -0.2356 (10) & 0.7660 (3) & 3.9 (2) \\ Co(1)-O(1) & 1.943 (8) & Co(2)-O(2) & 1.944 (7) & C(123) & 0.8286 (4) & -0.2305 (10) & 0.7660 (3) & 3.9 (2) \\ Co(1)-O(5) & 1.945 (7) & Co(2)-O(3) & 1.933 (7) & C(123) & 0.6386 (4) & -0.0350 (10) & 0.7660 (3) & 3.4 (2) \\ Co(1)-O(1) & 1.943 (8) & Co(2)-O(3) & 1.933 (7) & C(123) & 0.6387 (5) & -0.1663 (10) & 0.7021 (3) & 3.4 (2) \\ Co(1)-O(6) & 1.740 (1) & S(2)-C(22) & 1.72 (2) & C(133) & 0.6387 (5) & -0.1683 (10) & 0.5590 (4) & 6.03 \\ S(5)-C(25) & 1.73 (2) & S(3)-C(32) & 1.74 (1) & C(134) & 0.6335 (5) & -0.2867 (10) & 0.5560 (4) & 4.5 (2) \\ O(1)-N(1) & 1.34 (2) & O(2)-N(21) & 1.34 (1) & C(214) & 0.2867 (5) & -0.178 (10) & 0.5890 (4) & 6.03 \\ S(6)-C(66) & 1.70 (1) & S(4)-C(42) & 1.73 (2) & C(133) & 0.6393 (4) & -0.037 (10) & 0.5890 (4) & -0.017 (10) & 0.8499 (3) & 3.5 (2) \\ O(5)-N(51) & 1.38 (2) & O(3-N(31) & 1.35 (2) & C(213) & 0.8503 (5) & -0.3266 (10) & 0.5560 (4) & 4.5 (2) \\ O(5)-N(51) & 1.38 (2) & O(3-N(31) & 1.35 (2) & C(213) & 0.8503 (5) & -0.376 (10) & 0.5560 (4) & 4.5 (2) \\ O(5)-N(51) & 1.38 (2) & O(3-N(31) & 1.35 (2) & C(213) & 0.8593 (5) & -0.376 (10) & 0.5560 (4) & 4.5 (2) \\ O(5)-N(51) & 1.38 (2) & O(3-N(31) & 1.35 (2) & C(22) & 1.1202 (6) & 0.0176 (10) & 0.8999 (6) & 3.3 (2) \\ O(5)-N(51) & 1.38 (2) & O(3-N(31$	C(03) C(64)	0.4883 (10)	0.5931 (1	(0) 0.7167 (10) 0.7167 (10)	7.1 (5)	N(23)	0.5124(3)	0.3601 (7)	0.9325 (2)	2.8 (1)
$ \begin{array}{c} \hline C(66) & 0.5965 (10) & 0.6672 (8) & 0.5734 (9) & 3.7 (3) & (13) & (0.33) & (0.367) (8) & 0.7904 (2) & 2.9 (2) \\ C(112) & 0.8323 (4) & 0.5378 (10) & 0.6326 (3) & 2.8 (2) \\ C(113) & 0.8325 (4) & 0.5378 (10) & 0.6326 (4) & 3.9 (2) \\ C(113) & 0.8325 (4) & 0.5378 (10) & 0.6326 (4) & 4.9 (3) \\ C(113) & 0.8325 (4) & 0.5375 (10) & 0.5596 (4) & 4.9 (3) \\ C(113) & 0.8434 (5) & 0.5575 (10) & 0.5596 (4) & 4.9 (3) \\ C(11-S(1)) & 2.200 (4) & Co(2)-S(2) & 2.206 (3) & C(115) & 0.8379 (4) & 0.3594 (10) & 0.5521 (3) & 4.2 (2) \\ C(11-S(5)) & 2.199 (3) & Co(2)-S(3) & 2.200 (4) & C(122) & 0.8362 (4) & -0.2376 (10) & 0.7560 (3) & 3.9 (2) \\ Co(1)-S(5) & 2.208 (3) & Co(2)-S(3) & 2.201 (4) & C(122) & 0.8362 (4) & -0.2376 (10) & 0.7560 (3) & 3.9 (2) \\ Co(1)-C(1) & 1.943 (8) & Co(2)-O(2) & 1.944 (7) & C(124) & 0.9392 (4) & -0.3065 (10) & 0.7061 (3) & 3.9 (2) \\ Co(1)-O(6) & 1.943 (8) & Co(2)-O(3) & 1.932 (7) & C(133) & 0.6643 (4) & -0.0146 (10) & 0.5918 (3) & 3.3 (2) \\ Co(1)-O(6) & 1.943 (8) & Co(2)-O(3) & 1.732 (7) & C(133) & 0.6633 (4) & -0.0146 (10) & 0.5918 (3) & 3.3 (2) \\ Co(1)-O(6) & 1.943 (8) & Co(2)-O(3) & 1.74 (1) & C(132) & 0.6633 (4) & -0.0146 (10) & 0.5918 (4) & 5.4 (3) \\ S(5)-C(52) & 1.73 (2) & S(3)-C(32) & 1.74 (1) & C(134) & 0.6332 (5) & -0.1832 (10) & 0.5604 (4) & 5.4 (3) \\ S(5)-C(52) & 1.73 (2) & S(3)-C(32) & 1.74 (1) & C(134) & 0.6332 (5) & -0.1832 (10) & 0.5604 (4) & 5.4 (3) \\ S(6)-C(66) & 1.70 (1) & S(4)-C(42) & 1.73 (2) & C(133) & 0.6613 (6) & -0.0267 (10) & 0.5914 (4) & 5.4 (3) \\ S(6)-C(66) & 1.70 (1) & S(4)-C(42) & 1.73 (2) & C(133) & 0.6913 (5) & -0.2867 (10) & 0.5514 (4) & 5.4 (3) \\ S(6)-C(66) & 1.70 (1) & S(4)-C(42) & 1.73 (2) & C(134) & 0.6933 (5) & -0.1832 (10) & 0.5604 (4) & 5.4 (3) \\ S(6)-C(66) & 1.70 (1) & S(4)-C(2)-S(3) & 9.2 (1) & C(211) & 0.8573 (5) & -0.1832 (10) & 0.5806 (4) & 5.4 (3) \\ O(0)-N(61) & 1.38 (2) & O(3)-N(31) & 1.33 (2) & C(121) & 0.8573 (5) & -0.0177 (10) & 0.8499 (3) & 3.5 (2) \\ O(6)-N(61) & 1.38 (2) & O(3)-N(31) & 1.33 (2) & C(212) & 0.8573 (5) & -0.0177 (10) & 0.8499 (4) & 3.5 ($	C(65)	0.6620 (10)	0.6378 (1	0.6790 (10)	6.4 (5)	N(32)	0.4716 (3)	-0.0359(7)	0.8427 (3)	3.0 (2)
$ \begin{array}{c} C(111) \\ C(112) \\ C(112) \\ C(112) \\ C(113) \\ C(113) \\ C(113) \\ C(113) \\ C(113) \\ C(113) \\ C(114) \\ C(115) \\ C(11$	C(66)	0.5965 (10)	0.6672 (8	3) 0.5734 (9)	3.7 (3)	N(33)	0.3610 (3)	0.3877 (8)	0.7904 (2)	2.9 (2)
$\begin{array}{c} C(112) & 0.8323 (4) & 0.5378 (10) & 0.6334 (4) & 3.9 (2) \\ C(113) & 0.8525 (5) & 0.6119 (10) & 0.5591 (4) & 4.7 (8) \\ C(114) & 0.843 (5) & 0.5375 (10) & 0.5550 (4) & 4.9 (3) \\ C(115) & 0.8539 (4) & 0.3904 (10) & 0.5521 (3) & 4.2 (2) \\ C(1) & 0.211 (4) & -0.1356 (9) & 0.7170 (3) & 2.4 (2) \\ C(1) & 2.206 (3) & Co(2) & S(3) & 2.201 (4) & Co(123) & 0.8928 (4) & -0.0365 (10) & 0.7560 (3) & 3.9 (2) \\ C(1) & -0.056 (10) & 0.7560 (3) & 3.9 (2) \\ C(1) & -0.056 (10) & 0.7460 (3) & 3.9 (2) \\ C(1) & -0.051 (10) & 0.7480 (3) & 4.2 (2) \\ C(1) & -0.051 (10) & 0.7480 (3) & 2.201 (4) \\ C(1) & -0.051 (10) & 0.7480 (3) & 3.9 (2) \\ C(1) & -0.051 (10) & 0.7481 (3) & Co(2) & -0.03 \\ C(1) & -0.051 (10) & 0.7481 (3) & 0.7787 (4) & 4.6 (2) \\ C(1) & -0.051 (10) & 1.744 (1) & S(2) & -C(22) & 1.72 (2) \\ C(1) & -0.051 (10) & 1.744 (1) & S(2) & -C(22) & 1.744 (1) & C(113) & 0.6875 (5) & -0.1832 (10) & 0.5581 (4) & 5.4 (3) \\ S(5) & -C(52) & 1.73 (2) & S(3) & -C(32) & 1.744 (1) & C(133) & 0.8875 (5) & -0.2867 (10) & 0.5581 (4) & 5.4 (3) \\ S(6) & -C(66) & 1.70 (1) & S(4) & -C(42) & 1.73 (2) & C(123) & 0.6931 (5) & -0.2636 (10) & 0.5581 (4) & 5.4 (3) \\ O(1) & -N(11) & 1.34 (2) & O(2) & -N(21) & 1.344 (1) & C(211) & 0.5281 (5) & -0.178 (10) & 0.5499 (3) & 3.5 (2) \\ O(5) & -N(61) & 1.561 (0) & O(4) & -N(41) & 1.35 (2) & C(213) & 0.8533 (5) & -0.1386 (10) & 0.8130 (4) & 6.3 (3) \\ O(w) & -O(1m) & 2.79 (4) & C(22) & 1.1220 (4) & 0.0888 (10) & 0.9571 (4) & 6.5 (3) \\ O(w) & -O(1m) & 2.79 (4) & C(22) & 1.1230 (4) & 0.0888 (10) & 0.9571 (4) & 6.5 (3) \\ O(w) & -O(1m) & 2.79 (4) & C(22) & 1.1230 (4) & 0.0888 (10) & 0.9571 (4) & 6.5 (3) \\ O(1) & -C(1) & -S(6) & 9.2.1 (1) & S(2) & -C(2) & -S(3) & 9.2.0 (1) & -0.5831 (10) & 0.8937 (4) & 6.5 (3) \\ O(1) & -C(1) & -S(6) & 9.5.1 (1) & S(2) & -C(2) & -S(3) & 9.2.0 (1) & -0.5831 (10) & 0.8937 (4) & 6.5 (3) \\ O(1) & -C(1) & -S(6) & 9.5.1 (1) & S(2) & -C(2) & -O(3) & 9.3.0 (2) & C(223) & 1.1235 (4) & 0.0836 (10) & 0.9571 (4) & 6.5 (3) \\ O(1) & -C(1) & -S(6) & 9.5.1 (1) & S(2) & -C(2) & -O(3) & 9.3.0 (2) & C(2$						C(111)	0.8235 (4)	0.3851 (9)	0.6326 (3)	2.8 (2)
$\begin{array}{c} {\rm C(113)} & 0.3525 (5) & 0.6119 (10) & 0.3595 (4) & 4.7 (8) \\ {\rm C(114)} & 0.8643 (5) & 0.5375 (10) & 0.5550 (4) & 4.9 (3) \\ {\rm C(121)} & 0.8271 (4) & 0.3994 (10) & 0.5521 (3) & 4.2 (2) \\ {\rm C(1)-S(1)} & 2.206 (4) & {\rm C(2)-S(2)} & 2.208 (3) & {\rm C(122)} & 0.8378 (4) & -0.3356 (10) & 0.7550 (3) & 3.2 (2) \\ {\rm C(1)-S(1)} & 2.208 (3) & {\rm C(2)-S(3)} & 2.201 (4) & {\rm C(12)} & 0.8398 (4) & -0.3056 (10) & 0.7660 (3) & 3.9 (2) \\ {\rm C(1)-S(1)} & 2.208 (3) & {\rm C(2)-S(4)} & 2.213 (3) & {\rm C(124)} & 0.9399 (4) & -0.2024 (10) & 0.7402 (3) & 4.3 (2) \\ {\rm C(1)-O(5)} & 1.945 (7) & {\rm C(2)-O(3)} & 1.942 (7) & {\rm C(125)} & 0.9311 (4) & -0.1665 (10) & 0.7021 (3) & 3.4 (2) \\ {\rm C(1)-O(6)} & 1.945 (7) & {\rm C(2)-O(3)} & 1.942 (7) & {\rm C(133)} & 0.6688 (4) & -0.0302 (10) & 0.5797 (4) & 4.5 (2) \\ {\rm C(1)-O(6)} & 1.945 (7) & {\rm C(2)-C(22)} & 1.72 (2) & {\rm C(133)} & 0.6352 (5) & -0.1832 (10) & 0.5694 (4) & 6.0 (3) \\ {\rm S(5)-C(66)} & 1.70 (1) & {\rm S(4)-C(42)} & 1.73 (2) & {\rm C(133)} & 0.6352 (5) & -0.2867 (10) & 0.5541 (4) & 5.4 (3) \\ {\rm C(5)-N(51)} & 1.33 (2) & {\rm O(2)-N(11)} & 1.34 (1) & {\rm C(211)} & 0.9230 (4) & -0.0177 (10) & 0.8499 (3) & 3.5 (2) \\ {\rm O(6)-N(61)} & 1.36 (1) & {\rm O(4)-N(41)} & 1.35 (2) & {\rm C(213)} & 0.8503 (5) & 0.1736 (10) & 0.5818 (4) & 4.6 (2) \\ {\rm O(6)-N(61)} & 1.36 (1) & {\rm O(4)-N(41)} & 1.35 (2) & {\rm C(213)} & 0.8503 (5) & 0.1386 (10) & 0.8130 (4) & 6.3 (3) \\ {\rm O(w)- O(lm)} & 2.79 (4) & & & & & & & & & & & & & & & & & & &$						C(112)	0.8323 (4)	0.5378 (10)	0.6354 (4)	3.9 (2)
Table 2. Selected geometric parameters (Å, °) for (1) C(114) 0.8839 (4) 0.3331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) 0.5331 (10) <td></td> <td></td> <td></td> <td></td> <td></td> <td>C(113)</td> <td>0.8525 (5)</td> <td>0.6119 (10)</td> <td>0.5969 (4)</td> <td>4.7(8)</td>						C(113)	0.8525 (5)	0.6119 (10)	0.5969 (4)	4.7(8)
$ \begin{array}{c} \mbox{Label 2} Selected geometric parameters (x, -) for (1) \\ \mbox{Coll} 1 \\ \mbox{Coll} 2 \\ \mbox{Coll} 3 \\ \mbox{Coll} 2 \\ \mbox$		0 6			(1)	C(114)	0.8643 (5)	0.5375 (10)	0.5550 (4)	4.9 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Table	e 2. Selected	a geometric	c parameters (A,	-)]0/(1)	C(113)	0.8339 (4)	-0.1356 (9)	0.3321(3) 0.7170(3)	$\frac{4.2}{2.4}$ (2)
$ \begin{array}{c} Cot1 & -S(5) & 2.199 (3) & Cot2 & -S(3) & 2.201 (4) & Cot2 & 0.992 (4) & -0.305 (10) & 0.7660 (3) & 3.9 (2) \\ Cot1 & -S(6) & 2.208 (3) & Cot2 & -S(4) & 2.213 (3) & C(124) & 0.9399 (4) & -0.2624 (10) & 0.7402 (3) & 4.3 (2) \\ Cot1 & -O(1) & 1.943 (8) & Cot2 & -O(2) & 1.944 (7) & C(125) & 0.9311 (4) & -0.1665 (10) & 0.7402 (3) & 4.3 (2) \\ Cot1 & -O(6) & 1.943 (8) & Cot2 & -O(4) & 1.945 (7) & C(131) & 0.6648 (4) & -0.0146 (10) & 0.5918 (3) & 3.3 (2) \\ S(1) & -C(16) & 1.74 (1) & S(2) & -C(22) & 1.72 (2) & C(133) & 0.6638 (4) & -0.0502 (10) & 0.5599 (4) & 6.6 (3) \\ S(5) & -C(52) & 1.73 (2) & S(3) & -C(32) & 1.74 (1) & C(1134) & 0.6325 (5) & -0.1832 (10) & 0.5609 (4) & 6.0 (3) \\ S(6) & -C(66) & 1.70 (1) & S(4) & -C(42) & 1.73 (2) & C(133) & 0.6913 (5) & -0.2563 (10) & 0.5609 (4) & 4.5 (2) \\ O(1) & -N(11) & 1.34 (2) & O(2) - N(11) & 1.34 (1) & C(211) & 0.9280 (4) & -0.0177 (10) & 0.8499 (3) & 3.5 (2) \\ O(5) & -N(51) & 1.38 (2) & O(3) - N(31) & 1.33 (2) & C(213) & 0.8503 (5) & 0.1386 (10) & 0.8130 (4) & 6.3 (3) \\ O(w) & -O(ww) & 2.67 (3) & O(w) & -O(4) & 2.88 (1) & C(214) & 0.8935 (5) & 0.1386 (10) & 0.8130 (4) & 6.3 (3) \\ O(w) & -O(1m) & 2.79 (4) & C223 (1) & C223 (1) & 0.2935 (5) & 0.1951 (10) & 0.896 (4) & 5.0 (3) \\ S(1) & -Co(1) - S(6) & 92.2 (1) & S(2) - Co(2) - S(3) & 92.0 (1) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9935 (4) & 6.7 (3) \\ S(1) & -Co(1) - S(6) & 92.2 (1) & S(2) - Co(2) - S(3) & 92.0 (1) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9935 (4) & 6.5 (3) \\ S(1) & -Co(1) - O(6) & 17.5 (3) & S(2) - Co(2) - O(3) & 93.9 (2) & C(224) & 1.2427 (5) & 0.1748 (10) & 0.9837 (4) & 6.5 (3) \\ S(1) - Co(1) - O(6) & 17.5 (3) & S(2) - Co(2) - O(3) & 93.9 (2) & C(223) & 1.2085 (4) & -0.4329 (10) & 0.8784 (4) & 5.0 (3) \\ S(1) - Co(1) - O(6) & 17.5 (3) & S(2) - Co(2) - O(3) & 93.9 (2) & C(223) & 1.2085 (4) & -0.4329 (10) & 0.8784 (4) & 5.2 (3) \\ S(5) - Co(1) - O(6) & 17.5 (3) & S(2) - Co(2) - O(3) & 93.9 (2) & C(223) & 1.2085 (4) & -0.4329 (10) & 0.8784 (3) & 3.7 (2) \\ S(5) - Co(1) - O(6) & 17.5 (3) & S(2) - Co(2) - O(3)$	Co(1)—S	(1)	2.200 (4)	Co(2)—S(2)	2.208 (3)	C(121)	0.8368 (4)	-0.2376 (10)	0.7550 (3)	3.2 (2)
$ \begin{array}{c} Ca(1)-S(6) & 2.208 (3) \\ Ca(2)-S(6) & Ca(2)-S(4) \\ Ca(1)-O(5) & 1.943 (8) \\ Ca(2)-O(2) & 1.944 (7) \\ Ca(1)-O(6) & 1.943 (8) \\ Ca(2)-O(3) \\ Ca(1)-O(6) \\ 1.943 (8) \\ Ca(2)-O(3) \\ Ca(1)-O(6) \\ 1.943 (8) \\ Ca(2)-O(4) \\ 1.945 (7) \\ Ca(2)-O(3) \\ 1.92 (7) \\ Ca(131) \\ 0.6648 (4) \\ -0.0166 (10) \\ 0.0502 (10) \\ 0.0577 (4) \\ 4.6 (2) \\ S(5)-C(16) \\ 1.74 (1) \\ S(2)-C(22) \\ 1.72 (2) \\ Ca(133) \\ 0.6875 (5) \\ -0.2867 (10) \\ 0.5569 (4) \\ 0.556 (10) \\ 0.5569 (4) \\ 6.033 \\ (5)-C(56) \\ 1.70 (1) \\ S(4)-C(42) \\ 1.73 (2) \\ S(3)-C(56) \\ 1.70 (1) \\ S(4)-C(42) \\ 1.73 (2) \\ Ca(131) \\ 0.6325 (5) \\ -0.2867 (10) \\ 0.5563 (10) \\ 0.5569 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0556 (10) \\ 0.5560 (4) \\ 4.5 (2) \\ 0.0576 (4) \\ 4.5 (2) \\ 0.0576 (4) \\ 4.5 (2) \\ 0.0577 (4) \\ 4.5 (2) \\ 0.0578 (5) \\ 0.0176 (10) \\ 0.8898 (4) \\ 4.6 (2) \\ 0.0580 (10) \\ 0.880 (4) \\ 0.0808 (10) \\ 0.980 (4) \\ 4.5 (2) \\ 0.0808 (10) \\ 0.980 (4) \\ 0.980 (10) \\ 0.980 (4) \\ 0.993 (4) \\ 4.5 (2) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (2) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (3) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (3) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (3) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (3) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (3) \\ 0.0808 (10) \\ 0.993 (4) \\ 4.5 (3) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.0808 (10) \\ 0.993 (4) \\ 0.$	Co(1)—S	(5)	2.199 (3)	Co(2)—S(3)	2.201 (4)	C(123)	0.8928 (4)	-0.3005 (10)	0.7660 (3)	3.9 (2)
$ \begin{array}{c} Cot(1) = O(1) \\ Cot(1) = O(1) \\ Cot(1) = O(5) \\ 1.945 (7) \\ Cot(2) = O(3) \\ Cot(2) = O(3) \\ 1.932 (7) \\ Cr(13) \\ O(1) = O(6) \\ 1.943 (8) \\ Cot(2) = O(4) \\ 1.945 (7) \\ Cr(13) \\ O(1) = O(6) \\ 1.943 (8) \\ Cot(2) = O(4) \\ 1.945 (7) \\ Cr(13) \\ O(1) = O(6) \\ 1.74 (1) \\ S(2) = C(22) \\ 1.72 (2) \\ Cr(13) \\ O(1) = O(6) \\ 1.74 (1) \\ S(2) = C(22) \\ 1.72 (2) \\ Cr(13) \\ O(2) = O(25) \\ (1) \\ S(5) = C(52) \\ 1.73 (2) \\ S(3) = C(52) \\ 1.73 (2) \\ S(4) = C(4) \\ 1.73 (2) \\ O(2) = N(51) \\ 1.38 (2) \\ O(2) = N(51) \\ 1.38 (2) \\ O(2) = N(51) \\ 1.38 (2) \\ O(2) = N(31) \\ 1.38 (2) \\ O(3) = N(31) \\ 1.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38 (2) \\ 0.38$	Co(1)—S	(6)	2.208 (3)	Co(2) - S(4)	2.213 (3)	C(124)	0.9399 (4)	-0.2624 (10)	0.7402 (3)	4.3 (2)
$ \begin{array}{c} Cot1-O(5) & 1.943 (8) & Cot2-O(3) & 1.925 (7) & C(132) & 0.6648 (4) & -0.0146 (10) & 0.5918 (3) & 3.5 (2) \\ S(1)-C(16) & 1.74 (1) & S(2)-C(22) & 1.72 (2) & C(133) & 0.5875 (5) & -0.1832 (10) & 0.5609 (4) & 6.0 (3) \\ S(5)-C(52) & 1.73 (2) & S(3)-C(32) & 1.74 (1) & C(1134) & 0.6325 (5) & -0.2867 (10) & 0.5541 (4) & 5.4 (3) \\ S(6)-C(66) & 1.70 (1) & S(4)-C(42) & 1.73 (2) & C(135) & 0.6913 (5) & -0.2563 (10) & 0.5609 (4) & 4.5 (2) \\ O(1)-N(11) & 1.34 (2) & O(2)-N(21) & 1.34 (1) & C(211) & 0.9280 (4) & -0.0177 (10) & 0.8499 (3) & 3.5 (2) \\ O(5)-N(51) & 1.38 (2) & O(3)-N(31) & 1.33 (2) & C(212) & 0.8672 (5) & 0.0176 (10) & 0.8398 (4) & 4.6 (2) \\ O(6)-N(61) & 1.36 (1) & O(4)-N(41) & 1.35 (2) & C(213) & 0.8503 (5) & 0.1386 (10) & 0.8130 (4) & 6.3 (3) \\ O(w) \cdots O(ww) & 2.67 (3) & O(w) \cdots O(4) & 2.88 (1) & C(214) & 0.8945 (5) & 0.2289 (10) & 0.9770 (4) & 6.0 (3) \\ O(w) \cdots O(1m) & 2.79 (4) & C(221) & 1.1230 (4) & 0.0808 (10) & 0.9556 (3) & 3.3 (2) \\ S(1)-Co(1)-S(5) & 90.5 (1) & S(2)-Co(2)-S(3) & 92.0 (1) & C(222) & 1.1495 (5) & 0.174 (10) & 0.9925 (4) & 6.7 (3) \\ S(1)-Co(1)-O(5) & 92.6 (1) & S(2)-Co(2)-O(2) & 87.0 (2) & C(225) & 1.2185 (4) & 0.0826 (10) & 0.9281 (3) & 3.5 (2) \\ S(1)-Co(1)-O(5) & 92.6 (2) & S(2)-Co(2)-O(2) & 87.0 (2) & C(225) & 1.2185 (4) & 0.0826 (10) & 0.9287 (4) & 6.5 (3) \\ S(1)-Co(1)-O(5) & 92.6 (2) & S(2)-Co(2)-O(4) & 97.0 (2) & C(225) & 1.2185 (4) & 0.0826 (10) & 0.9287 (4) & 5.2 (3) \\ S(5)-Co(1)-O(5) & 91.1 (1) & S(3)-Co(2)-O(4) & 91.1 (2) & C(233) & 1.1115 (6) & -0.6614 (10) & 0.8415 (4) & 5.9 (3) \\ S(5)-Co(1)-O(5) & 91.2 (2) & S(3)-Co(2)-O(4) & 91.1 (2) & C(233) & 1.1023 (5) & -0.5819 (10) & 0.8784 (3) & 3.7 (2) \\ S(5)-Co(1)-O(6) & 91.7 (2) & S(4)-Co(2)-O(3) & 173.7 (2) & C(312) & 0.5246 (5) & 0.2609 (10) & 0.9966 (4) & 5.2 (3) \\ S(5)-Co(1)-O(6) & 87.7 (2) & S(4)-Co(2)-O(3) & 173.7 (2) & C(312) & 0.5246 (5) & 0.2609 (10) & 0.9966 (4) & 5.2 (3) \\ S(5)-Co(1)-O(6) & 87.7 (2) & S(4)-Co(2)-O(3) & 173.7 (2) & C(312) & 0.5246 (5) & 0.2609 (10) & 0.9966 (4) & 5.2 (3) \\ S(6)-Co(1)-O(6) & 87.7 (4) & O($	$C_0(1) - C_0(1)$	D (1)	1.943 (8)	$C_0(2) = O(2)$	1.944 (7)	C(125)	0.9311 (4)	-0.1665 (10)	0.7021 (3)	3.4 (2)
$\begin{array}{c} Cu(1) = 0.00 & 1.74 (1) & S(2) = C(2) & 1.72 (2) & 0.6036 (4) & -0.030 (10) & 0.379 (4) & 4.8 (2) \\ S(3) = C(52) & 1.73 (2) & S(3) = C(32) & 1.74 (1) & C(133) & 0.6325 (5) & -0.1832 (10) & 0.5609 (4) & 6.0 (3) \\ S(5) = C(56) & 1.70 (1) & S(4) = C(42) & 1.73 (2) & C(133) & 0.6325 (5) & -0.2867 (10) & 0.5541 (4) & 5.4 (3) \\ S(6) = C(66) & 1.70 (1) & S(4) = C(42) & 1.73 (2) & 0.6913 (5) & -0.2563 (10) & 0.560 (4) & 4.5 (2) \\ O(1) = N(11) & 1.34 (2) & O(2) = N(21) & 1.34 (1) & C(211) & 0.9280 (4) & -0.0177 (10) & 0.8499 (3) & 3.5 (2) \\ O(6) = N(61) & 1.36 (1) & O(4) = N(41) & 1.33 (2) & C(212) & 0.8672 (5) & 0.0176 (10) & 0.8398 (4) & 4.6 (2) \\ O(6) = N(61) & 1.36 (1) & O(4) = N(41) & 1.33 (2) & C(213) & 0.8503 (5) & 0.1386 (10) & 0.8130 (4) & 6.3 (3) \\ O(w) = O(1ww) & 2.67 (3) & O(w) = O(4) & 2.88 (1) & C(214) & 0.8945 (5) & 0.2289 (10) & 0.7970 (4) & 6.0 (3) \\ O(w) = O(6) & 2.88 (1) & O(ww) = O(5) & 2.95 (3) & C(215) & 0.9533 (5) & 0.1951 (10) & 0.8966 (4) & 5.0 (3) \\ O(w) = O(1) = S(5) & 90.5 (1) & S(2) = Co(2) = S(3) & 92.0 (1) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9950 (3) & 3.3 (2) \\ S(1) = Co(1) = S(6) & 92.2 (1) & S(2) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.7 (3) \\ S(1) = Co(1) = O(6) & 175.5 (3) & S(2) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.7 (3) \\ S(1) = Co(1) = O(6) & 175.5 (3) & S(2) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.7 (3) \\ S(5) = Co(1) = O(6) & 175.5 (3) & S(2) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.7 (3) \\ S(5) = Co(1) = O(6) & 175.5 (3) & S(2) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.7 (3) \\ S(5) = Co(1) = O(6) & 175.5 (3) & S(2) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.5 (3) \\ S(5) = Co(1) = O(6) & 174.9 (3) & S(3) = Co(2) = O(3) & 93.9 (2) & C(223) & 1.2076 (6) & 0.2171 (10) & 0.9951 (4) & 6.7 (3) \\ S(5) = Co(1) = O(6) & 174.9 (3) & S(3) = Co(2) = O(3)$	$C_0(1) = C_0(1) = C$)(5))(6)	1.943 (7)	$C_0(2) = O(3)$	1.945 (7)	C(131)	0.6648 (4)	-0.0146 (10)	0.5918 (3)	3.3(2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		16)	1.943(0)	S(2) - C(22)	1.72 (2)	C(132)	0.6036 (4)	-0.0502(10)	0.5797 (4)	4.0(2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	S(5) - C(52)	1.73 (2)	S(3) - C(32)	1.74 (1)	C(133)	0.5875 (5)	-0.1852(10) -0.2867(10)	0.5609(4)	5.4 (3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	S(6)—C(66)	1.70 (1)	S(4)—C(42)	1.73 (2)	C(135)	0.6913 (5)	-0.2563(10)	0.5660 (4)	4.5 (2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	O(1)N	(11)	1.34 (2)	O(2)—N(21)	1.34 (1)	C(211)	0.9280 (4)	-0.0177 (10)	0.8499 (3)	3.5 (2)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(5)—N	(51)	1.38 (2)	O(3)—N(31)	1.33 (2)	C(212)	0.8672 (5)	0.0176 (10)	0.8398 (4)	4.6 (2)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(6)—N	(61)	1.36 (1)	O(4) - N(41)	1.35 (2)	C(213)	0.8503 (5)	0.1386 (10)	0.8130 (4)	6.3 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$O(w) \cdots O(w) \cdots O(w)$	U(ww)	2.67 (3)	$O(w) \cdots O(4)$	2.88 (1)	C(214)	0.8945 (5)	0.2289 (10)	0.7970 (4)	6.0 (3)
$\begin{array}{c} C(21) & (1,23) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) & (2,1) $	$O(w) \cdots O(w)$	J(0) .O(1m)	2.00(1)	$O(ww) \cdots O(J)$	2.95 (5)	C(215)	0.9535 (5)	0.1951 (10)	0.8066 (4)	3.0(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0(ww).	•0(1m)	2.75 (4)		02.0 (1)	C(221)	1.1230 (4)	0.0808 (10)	0.9300 (3)	3.3(2) 45(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(1)—Co	S(1) = S(5)	90.5 (1)	S(2) = Co(2) = S(3) S(2) = Co(2) = S(4)	92.0(1)	C(222)	1.1495 (5)	0.2171 (10)	0.9935 (4)	6.7 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$S(1) \rightarrow C(1)$	S(1) = S(0)	92.2 (1)	S(2) = CO(2) = S(4) S(2) = CO(2) = O(2)	87.0 (2)	C(223)	1.2427 (5)	0.1748 (10)	0.9587 (4)	6.5 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		(1) = 0(1)	92.6 (2)	S(2) - Co(2) - O(3)	93.9 (2)	C(225)	1.2185 (4)	0.0826 (10)	0.9231 (3)	5.2 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$S(1) \rightarrow C(1)$	(1) - O(6)	175.5 (3)	S(2)-Co(2)-O(4)	174.9 (3)	C(231)	1.0859 (4)	-0.4329 (10)	0.8784 (3)	3.7 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(5)—Co	o(1)—S(6)	91.1 (1)	S(3)—Co(2)—S(4)	91.1 (1)	C(232)	1.1023 (5)	-0.5819 (10)	0.8823 (4)	5.1 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(5)—Co	o(1)O(1)	176.0 (2)	S(3)-Co(2)-O(2)	176.8 (2)	C(233)	1.1115 (6)	-0.6614 (10)	0.8415 (4)	5.9 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	S(5)—Co	o(1)—O(5)	87.2 (2)	S(3)—Co(2)—O(3)	87.4 (3)	C(234)	1.1072 (5)	0.5943 (10)	0.7900 (4)	3.2(3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	S(5)—Co	o(1)O(6)	94.0 (2)	S(3) - Co(2) - O(4)	93.1 (2)	C(235)	1.0909 (5)	-0.4509(10)	0.7920(4)	$\frac{4.3}{32}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(6)—C	O(1) - O(1)	92.6 (2)	S(4) = Co(2) = O(2) S(4) = Co(2) = O(2)	92.1 (2) 173 7 (2)	C(312)	0.5246(5)	0.2603 (10)	1.0110 (3)	4.3 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(6)-C	u(1) = 0(3)	1 /4.7 (3) 87 7 (7)	S(4) = Co(2) = O(3)	87.6 (2)	C(313)	0.5734 (5)	0.3490 (10)	1.0241 (3)	4.7 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0(1)	(1) - O(5)	89.2 (4)	O(2) - Co(2) - O(3)	89.6 (3)	C(314)	0.5920 (4)	0.4457 (10)	0.9897 (4)	4.3 (2)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0(1)-C	o(1)O(6)	87.8 (3)	O(2)-Co(2)-O(4)	88.0 (3)	C(315)	0.5612 (4)	0.4483 (10)	0.9443 (3)	3.6 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(5)—C	o(1)O(6)	87.7 (4)	O(3)-Co(2)-O(4)	86.3 (3)	C(321)	0.5194 (4)	-0.1257 (10)	0.8363 (4)	4.0 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Co(1)	S(1)—C(16)	96.7 (4)	Co(2)—S(2)—C(22)	96.6 (4)	C(322)	0.5092 (5)	-0.2724 (10)	0.8299 (4)	5.5 (5) 5.7 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Co(1)	S(5)—C(52)	96.2 (4)	Co(2)— $S(3)$ — $C(32)$	96.2 (4)	C(323)	0.4508 (5)	-0.3273(10) -0.2354(10)	0.8303 (4)	J.2 (J) 4 5 (J)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Co(1)	S(6)—C(66)	97.1 (4)	Co(2) = S(4) = C(42)	95.7 (4) 116.0 (6)	C(324) C(325)	0.4037 (3)	-0.0852 (10)	0.8421 (3)	3.1 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{\alpha}(1)$	O(1) - N(11) O(5) - N(51)	110.3 (0)	$C_0(2) = O(2) = N(21)$ $C_0(2) = O(3) = N(31)$	118.1 (6)	C(331)	0.3229 (4)	0.4249 (10)	0.8243 (3)	3.1 (2)
	Co(1)	O(6) - N(61)	115.7 (6)	Co(2) - O(4) - N(41)	115.2 (6)	C(332)	0.2719 (4)	0.5092 (10)	0.8083 (4)	4.4 (2)

C(333)	0.2614 (5)	0.5508	(10)	0.7609 (4)	5.8 (3)
C(334)	0.3008 (5)	0.5101	(10)	0.7277 (4)	5.6 (3)
C(335)	0.3514 (4)	0.4297	(10)	0.7434 (3)	4.0 (2)
O(<i>m</i>)	1.2312 (5)	-0.2829	(10)	0.8951 (4)	12.4 (3)
C(<i>m</i>)	1.2496 (9)	-0.3262	(3)	0.9458 (7)	16.2 (7)
					• • •
		_		0	
Table	4. Selected	d geometr	ic para	meters (A, °)) for (2)
Co(1)—S(11)	2.214 (2)	S(21)-	-C(211)	1.728 (8)
Co(1)—S(12)	2.203 (2)	S(22)–	-C(221)	1.724 (8)
Co(1)—S(13)	2.202 (2)	S(23)-	-C(231)	1.731 (9)
Co(1)—O((11)	1.976 (5)	O(21)-	—N(21)	1.336 (8)
Co(1)—O((12)	1.954 (5)	O(22)-	—N(22)	1.360 (8)
Co(1)—O((13)	1.951 (6)	O(23)-	—N(23)	1.352 (8)
S(11)—C(111)	1.710 (8)	Co(3)-	–S(31)	2.205 (2)
S(12)—C(121)	1.735 (7)	Co(3)-	–S(32)	2.206 (2)
S(13)—C(131)	1.724 (8)	Co(3)-	–S(33)	2.207 (2)
O(11)—N((11)	1.348 (8)	Co(3)-	O(31)	1.945 (6)
O(12)—N((12)	1.357 (8)	Co(3)-	O(32)	1.927 (6)
O(13)—N((13)	1.343 (8)	Co(3)-	-O(33)	1.943 (5)
$O(22) \cdot \cdot \cdot C$	$\mathcal{P}(m)$	2.91 (1)	S(31)–	-C(311)	1.734 (8)
Co(2)—S(21)	2.190 (2)	S(32)–	-C(325)	1.728 (9)
Co(2)—S(22)	2.204 (2)	S(33)–	-C(331)	1.718 (9)
Co(2)—S(23)	2.215 (2)	O(31)-	—N(31)	1.349 (7)
Co(2)—O((21)	1.938 (5)	O(32)-	—N(32)	1.348 (7)
Co(2)O((22)	1.967 (5)	O(33)-	—N(33)	1.348 (7)
Co(2)O((23)	1.946 (5)			
S(11)—Co	(1)—O(11)	87.0 (2)	Co(2)-	-\$(23)-C(231)	96.9 (3)
S(12)—Co	o(1)—O(12)	87.9 (2)	Co(2)-	O(21)N(21)	115.8 (5)
S(13)—Co	o(1)O(13)	86.6 (2)	Co(2)-	-O(22)-N(22)	115.7 (4)
Co(1)—S(11)—C(111)	96.9 (3)	Co(2)-	-O(23)-N(23)	116.9 (4)
Co(1)—S(12)—C(121)	96.9 (2)	S(31)-	-Co(3)O(31)	87.3 (2)
Co(1)—S(13)—C(131)	97.5 (3)	S(32)-	-Co(3)O(32)	88.0 (2)
Co(1)O((11)—N(11)	115.1 (5)	S(33)-	-Co(3)-O(33)	87.1 (2)
Co(1)O((12)—N(12)	116.1 (4)	Co(3)-	-S(31)-C(311)	97.1 (3)
Co(1)O((13)—N(13)	114.7 (4)	Co(3)-	-S(32)-C(325)	96.3 (2)
S(21)—Co	o(2)O(21)	87.8 (2)	Co(3)-	-S(33)-C(331)	96.8 (3)
S(22)—Co	o(2)—O(22)	87.5 (2)	Co(3)-	O(31)N(31)	116.4 (5)
S(23)—Co	o(2)—O(23)	87.5 (2)	Co(3)-	-O(32)N(32)	115.6 (4)
Co(2)-S(21)—C(211)	97.4 (3)	Co(3)-	-O(33)-N(33)	116.1 (4)

The H atoms, except those of H_2O and MeOH for (1) and MeOH for (2), were placed at calculated positions and given isotropic displacement factors derived from those of the parent atoms. The H atoms were included in the structure-factor calculations but not refined. Both structures were solved by direct methods (Main *et al.*, 1982) and refined by full-matrix least squares (Frenz, 1985).

98.1 (2)

Co(2)-S(22)-C(221)

We appreciate very much the financial support from the Climbing Program – National Key Project for Fundamental Research, the NNSF of China and the NSF of the Province of Fujian.

Lists of structure factors, anisotropic displacement parameters, Hatom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1088). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Chen, X.-T., Hu, Y.-H., Weng, L.-H., Xu, Y.-J., Wu, D.-X. & Kang, B.-S. (1991). Polyhedron, 10, 2651-2657.
- Cromer, D. T. & Waber, J. T. (1974). International Tables for X-ray Crystallography, Vol. IV, Table 2.2B. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

© 1995 International Union of Crystallography Printed in Great Britain – all rights reserved

- Frenz, B. A. (1985). Enraf-Nonius SDP-Plus Structure Determination Package. Version 3.0. Enraf-Nonius, Delft, The Netherlands.
- Hu, Y.-H., Weng, L.-H., Huang, L.-R., Chen, X.-T., Wu, D.-X. & Kang, B.-S. (1991). Acta Cryst. C47, 2655–2656.
- Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Kang, B.-S., Hu, Y.-H., Weng, L.-H., Wu, D.-X., Chen, X.-T. & Xu, Y.-J. (1992). J. Inorg. Biochem. 46, 231-242.
- Kang, B.-S., Peng, J.-H., Hong, M.-C., Wu, D.-X., Chen, X.-T., Weng, L.-H., Lei, X.-J. & Liu, H.-Q. (1991). J. Chem. Soc. Dalton Trans. pp. 2897–2901.
- Kang, B.-S., Weng, L.-H., Liu, H.-Q., Wu, D.-X., Huang, L.-R., Lu, C.-Z., Cai, J.-H., Chen, X.-T. & Lu, J.-X. (1990). *Inorg. Chem.* 29, 4073–4077.
- Kang, B.-S., Weng, L.-H., Wu, D.-X., Wang, F., Guo, Z., Huang, L.-R., Huang, Z.-Y. & Liu, H.-Q. (1988). *Inorg. Chem.* 27, 1128–1130.
- Kang, B.-S., Xu, Y.-J., Peng, J.-H., Wu, D.-X., Chen, X.-T., Hu, Y.-H., Hong, M.-C. & Lu, J.-X. (1993). Polyhedron, 12, 871–878.
- Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1982). MULTAN11/82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data. Univs. of York, England, and Louvain, Belgium.

Acta Cryst. (1995). C51, 374-377

Two-Dimensional Open-Frame Host Structure of the Inclusion Compound $[Cd(tenH)_2{Ni(CN)_4}_2].4C_6H_5NH_2$ (ten = 1,4-Diazabicyclo[2.2.2]octane)

HIDETAKA YUGE AND TOSCHITAKE IWAMOTO

Department of Chemistry, College of Arts and Sciences, The University of Tokyo, Komaba, Meguro, Tokyo 153, Japan

(Received 10 May 1994; accepted 11 August 1994)

Abstract

In the title inclusion compound, bis(1-azonia-4azabicyclo[2.2.2]octane)cadmium(II) bis[tetracyanonickelate(II)]-aniline (1/4), $[Cd(C_6H_{13}N_2)_2{Ni(CN)_4}_2]$.- $4C_6H_7N$, the host contains Cd^{2+} and $[Ni(CN)_4]^{2-}$ in a ratio of 1:2. The two crystallographically independent $[Ni(CN)_4]^{2-}$ anions behave as bidentate bridging ligands, spanning the Cd^{2+} cations with the N atoms of the cyano groups in *trans* positions along both the *a* and *b* axes, building up a two-dimensional network $[Cd(tenH)_2{NC-Ni(CN)_2-CN-}_2]_n$ (ten = 1,4diazabicyclo[2.2.2]octane). Two unidentate tenH ligands coordinate to the Cd in axial positions, the other Natom end being protonated. The guest aniline molecules accommodated in the interlayer space are hydrogen