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

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Co	0	0	0	0.03247 (15)
N1	0.1254 (2)	−0.1208 (2)	−0.40919 (9)	0.0291 (3)
N2	−0.2178 (2)	−0.3233 (2)	−0.46806 (9)	0.0318 (3)
N3	−0.1666 (2)	−0.1890 (2)	−0.32340 (9)	0.0305 (3)
N4	0.0532 (2)	−0.2706 (2)	−0.55340 (9)	0.0343 (3)
N5	0.4308 (3)	−0.1303 (3)	−0.58812 (11)	0.0448 (4)
N6	−0.5071 (2)	−0.4085 (2)	−0.39117 (10)	0.0348 (3)
N7	−0.6882 (3)	−0.4157 (4)	−0.25941 (13)	0.0595 (5)
N8	0.1924 (2)	0.0130 (2)	−0.27037 (9)	0.0335 (3)
N9	0.0941 (3)	0.0406 (3)	−0.12382 (10)	0.0410 (4)
C1	−0.0045 (2)	−0.2361 (2)	−0.47826 (10)	0.0276 (3)
C2	−0.2961 (3)	−0.3043 (3)	−0.39084 (10)	0.0285 (3)
C3	0.0444 (3)	−0.0998 (3)	−0.33228 (10)	0.0275 (3)
C4	0.2583 (3)	−0.1910 (3)	−0.56789 (10)	0.0321 (4)
C5	−0.5942 (3)	−0.4071 (3)	−0.31829 (13)	0.0386 (4)
C6	0.1288 (3)	0.0247 (3)	−0.19346 (11)	0.0322 (4)
O1	0.1928 (3)	0.3137 (2)	0.04206 (11)	0.0513 (4)
O2	0.2639 (3)	−0.0793 (3)	0.03380 (10)	0.0512 (4)
O3	0.3538 (2)	−0.0720 (3)	0.20893 (9)	0.0459 (3)
O4	−0.3540 (3)	0.3773 (3)	0.06728 (12)	0.0583 (4)
O5	0.1018 (4)	−0.4960 (3)	0.1794 (2)	0.0792 (6)

Table 2. *Selected geometric parameters* (Å, °)

Co—O2	2.062 (2)	N4—C1	1.305 (2)
Co—N9	2.092 (2)	N4—C4	1.319 (2)
Co—O1	2.107 (2)	N5—C4	1.149 (2)
N1—C1	1.351 (2)	N6—C5	1.324 (2)
N1—C3	1.382 (2)	N6—C2	1.327 (2)
N2—C1	1.355 (2)	N7—C5	1.148 (3)
N2—C2	1.375 (2)	N8—C6	1.319 (2)
N3—C2	1.331 (2)	N8—C3	1.319 (2)
N3—C3	1.337 (2)	N9—C6	1.143 (2)
O2—Co—N9^{i}	90.39 (7)	N4—C1—N1	127.07 (14)
O2—Co—N9	89.62 (7)	N4—C1—N2	116.91 (14)
O2—Co—O1	88.10 (8)	N1—C1—N2	116.01 (14)
N9—Co—O1	91.57 (7)	N6—C2—N3	124.72 (15)
O2—Co—O1^{i}	91.90 (8)	N6—C2—N2	113.98 (15)
N9—Co—O1^{i}	88.43 (7)	N3—C2—N2	121.30 (14)
C1—N1—C3	121.43 (14)	N8—C3—N3	124.33 (15)
C1—N2—C2	122.01 (14)	N8—C3—N1	114.14 (14)
C2—N3—C3	117.62 (14)	N3—C3—N1	121.53 (14)
C1—N4—C4	120.23 (14)	N5—C4—N4	173.7 (2)
C5—N6—C2	117.98 (15)	N7—C5—N6	173.6 (2)
C6—N8—C3	117.23 (14)	N9—C6—N8	173.4 (2)
C6—N9—Co	167.8 (2)		

Symmetry code: (i) $-x, -y, -z$.

The structure was solved using the *TREF* routine in *SHELXS*86 (Sheldrick, 1990). Refinement was performed using *SHELXL*93 (Sheldrick, 1993). All non-H atoms were refined with anisotropic displacement parameters. H atoms were refined isotropically. The water H atoms were refined with a common O—H separation. The tables were produced using *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1099). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tetrakis(creatinine)platinum(II) Dithiocyanate

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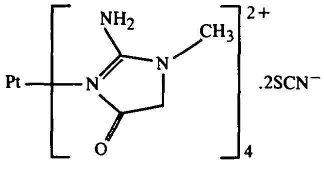
Abstract

The structure of the title compound, tetrakis(2-amino-1,5-dihydro-1-methyl-4*H*-imidazol-4-one-N^3)platinum(II) dithiocyanate, $[Pt(C_4H_7N_3O)_4](SCN)_2$, consists of $[Pt(creat)_4]^{2+}$ (creat is 2-imino-1-methyl-4-imidazolidinone) complex cations possessing approximate D_2 symmetry and thiocyanate anions. The Pt atom is coordinated in a square-planar manner by four creatinine ligands bonded through their endocyclic N atoms. The Pt—N bond distances range from 1.980 (6) to 2.034 (7) Å. The creatinine molecules are planar and participate in inter- and intramolecular hydrogen bonds. The ligands are almost perpendicular to the equatorial PtN_4 plane.

Comment

Recently, a number of structural papers on different Pt^{II}–creatinine complexes have appeared (Mitewa, Gencheva, Bontchev & Macíček, 1988; Macíček, Angelova, Gencheva, Mitewa & Bontchev, 1988; Beurskens, Perales, Martin-Gil & Martin-Gil, 1988; Beja, Paixao, Martin-Gil & Salgado, 1991; Gencheva *et al.*, 1992). It was found that changing the reaction conditions led to the formation of different complex species, some of them being paramagnetic metal–metal-bonded and creatinine-bridged oligomers involving Pt^{III}, as in the 'platinum blues', *i.e.* compounds with potential antitumor activity (Martin-Gil & Martin-Gil, 1987; Bontchev, Mitewa & Gencheva, 1989; Geraldes, Aragon-Salgado & Martin-Gil, 1991; Gencheva, Mitewa & Bontchev, 1992; Coronado, Gomez-Garcia, Martin-Gil & Martin-Gil, 1992; Mitewa, 1995). The structure of the Pt^{II}–creatinine and mixed-valence Pt^{II}/Pt^{III}–creatinine complexes, together with the coordination mode of the ligand, have been investigated by X-ray, spectroscopic and magnetochemical techniques in order to study the interaction of the Pt atom in different oxidation states with this biologically important ligand.

The title tetrakis(creatinine)platinum(II) dithiocyanate complex salt, (I), was obtained by interaction of Pt^{IV} (as $PtCl_6^{2-}$) and creatinine in water solution (pH < 3) and was isolated with thiocyanate anions. The primary analytical and spectroscopic [IR, ^1H NMR, ESCA (electron spectroscopy for chemical analysis) and EPR (electron paramagnetic resonance)] data indicated the formation of the creatinine complex of Pt^{II} as a final product, *i.e.* $[Pt(creat)_4]^{2+}$ (Mitewa, Gencheva, Simova & Nefedov, 1991). This complex is also the final product of the $Pt^{II}Cl_4^{2-}$–creatinine reaction in water solution. A redox interaction therefore takes place between Pt^{IV} and creatinine in water solution and it can be supposed that creatinine acts as a reducing agent. The reduction properties of creatinine are not unexpected because during an investigation of the pulsed photolysis of the $Pt^{IV}Cl_6^{2-}$–creatinine–methanol system, the reduction of Pt^{IV} to Pt^{II} and the formation of the $[Pt^{II}(creat)_4]^{2+}$ complex cation were proved (Grivin *et al.*, 1990). The existence of the Cu^{I}–creatinine complex obtained from the interaction of Cu^{II} with creatinine has also been reported (Birdsall & Weber, 1990).



(I)

The crystal structure consists of $[Pt(creat)_4]^{2+}$ complex cations (Fig. 1) with D_2 symmetry and thiocyanate anions. The Pt atom is coordinated in a square-planar manner by the *endo*-N atoms of four creatinine ligands. The Pt—N distances range from 1.980 (6) to 2.034 (7) Å and the adjacent N1—Pt—N1 angles vary between 89.1 (3) and 91.8 (3)°. The creatinine molecules are almost planar and their bond lengths and angles are typical. The creatinine molecules are planar within 0.01 (1), 0.09 (1), 0.03 (1) and 0.04 (1) Å for the *a*, *b*, *c* and *d* molecules, respectively, and are tilted with respect to the PtN_4 coordination plane by 91.8 (2), 73.9 (2), 93.0 (2) and 86.5 (2)°.

The SCN^- anion lies in the cavity formed by four creatinine molecules coordinated in pairs to two different Pt atoms (Fig. 2). The S—C and C—N bond lengths are 1.595 (11) and 1.104 (15), and 1.636 (12) and 1.115 (15) Å for the first and second ion, respectively, with S—C—N angles of 178 (1) and 179 (2)°.

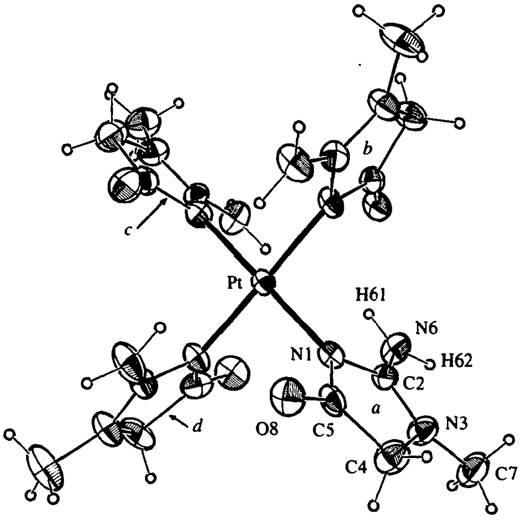


Fig. 1. A view of the complex cation of (I) with the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms have been arbitrarily reduced.

The cations are held together by a network of hydrogen bonds involving all the amino groups and three of the carbonyl groups (Fig. 2). The *a* and *c* amino groups are hydrogen bonded to atom O8*b*($-x$, $1-y$, $1-z$) [N6*a*···O8*b* 3.047 (9), N6*c*···O8*b* 2.837 (11) Å and N6*a*···O8*b*···N6*c* 108.6 (3)°]. The *b* amino group takes part in both an intramolecular hydrogen bond with the *c* carbonyl group [N6*b*···O8*c* 2.931 (9) Å] and an

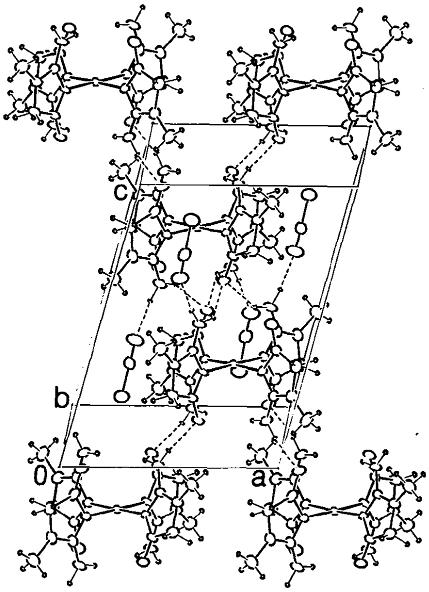


Fig. 2. An *ac* projection of the title structure. Dashed lines denote hydrogen bonds.

intermolecular hydrogen bond [N6*b*···O8*c*($-x$, $1-y$, $-z$) 2.861 (9) Å]. The N6*d* atom is hydrogen-bonded to the O8*a*($1-x$, $1-y$, $-z$) atom only [2.827 (8) Å]. There are also two hydrogen bonds to the thiocyanate N atoms [N6*a*···N1 2.864 (14) and N6*c*···N2($1-x$, $1-y$, $1-z$) 2.923 (10) Å].

Experimental

Crystals suitable for X-ray analysis were obtained after a few days from a reaction mixture consisting of $(NH_4)_2PtCl_6$ (1 mmol, Fluka) dissolved in HCl (0.1 mol) and aqueous solutions of creatinine (8 mmol, Fluka) and KSCN (8 mmol, Merck) at ambient temperature.

Crystal data

$[Pt(C_4H_7N_3O)_4](SCN)_2$
$M_r = 763.73$
Triclinic
$P\overline{1}$
$a = 10.372\ (3)$ Å
$b = 10.787\ (2)$ Å
$c = 13.571\ (3)$ Å
$\alpha = 74.35\ (2)°$
$\beta = 74.37\ (2)°$
$\gamma = 87.03\ (2)°$
$V = 1407.6\ (7)$ Å^3
$Z = 2$
$D_x = 1.801$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 22 reflections
$\theta = 19.96–21.55°$
$\mu = 5.22$ mm^{-1}
$T = 292$ K
Elongated
0.28 × 0.26 × 0.24 mm
Transparent

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scans (North, Phillips & Mathews, 1968)
$T_{\min} = 0.861$, $T_{\max} = 0.998$
4696 measured reflections
4417 independent reflections

3691 observed reflections [$I > 3\sigma(I)$]
$R_{\rm int} = 0.021$
$\theta_{\max} = 24°$
$h = 0 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 120 min
intensity decay: 2.1%

Refinement

Refinement on F
$R = 0.034$
$wR = 0.046$
$S = 0.884$
3691 reflections
352 parameters
H atoms refined as riding
$w = 1/[\sigma^2(F) + (0.04F)^2]$

$(\Delta/\sigma)_{\max} = 0.208$
$\Delta\rho_{\max} = 1.86$ e Å^{-3} (near Pt)
$\Delta\rho_{\min} = -1.98$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *SDP/PDP* (Enraf–Nonius, 1985)

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

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Pt	0.17071 (3)	0.44481 (3)	0.27035 (2)	0.03069 (8)
S1	0.2988 (3)	0.5498 (3)	0.8495 (2)	0.089 (1)
C1	0.3057 (9)	0.5596 (10)	0.7288 (7)	0.065 (3)
N1	0.3105 (11)	0.5693 (13)	0.6448 (7)	0.144 (6)
S2	0.2181 (4)	0.9583 (4)	0.1326 (3)	0.108 (1)
C2	0.2048 (10)	0.9500 (10)	0.2571 (8)	0.069 (4)
N2	0.1961 (11)	0.9428 (10)	0.3422 (7)	0.115 (5)
N1*a*	0.3047 (6)	0.5764 (6)	0.2688 (5)	0.041 (2)
C2*a*	0.3335 (8)	0.6000 (8)	0.3530 (7)	0.049 (3)
N3*a*	0.4341 (7)	0.6857 (7)	0.3221 (6)	0.059 (3)
C4*a*	0.4824 (9)	0.7256 (9)	0.2077 (7)	0.066 (3)
C5*a*	0.3890 (8)	0.6470 (8)	0.1729 (7)	0.051 (3)
N6*a*	0.2689 (7)	0.5446 (7)	0.4507 (5)	0.065 (3)
C7*a*	0.491 (1)	0.7331 (10)	0.3924 (7)	0.090 (4)
O8*a*	0.3897 (6)	0.6441 (6)	0.0861 (4)	0.062 (2)
N1*b*	0.0368 (6)	0.5828 (6)	0.2572 (4)	0.032 (2)
C2*b*	−0.0014 (8)	0.6445 (7)	0.1653 (6)	0.035 (2)
N3*b*	−0.0882 (7)	0.7375 (6)	0.1780 (5)	0.046 (2)
C4*b*	−0.1084 (9)	0.7524 (9)	0.2848 (6)	0.056 (3)
C5*b*	−0.0250 (8)	0.6451 (8)	0.3283 (6)	0.040 (2)
N6*b*	0.0440 (7)	0.6127 (7)	0.0762 (5)	0.048 (2)
C7*b*	−0.1319 (9)	0.8301 (9)	0.0967 (7)	0.067 (3)
O8*b*	−0.0157 (6)	0.6152 (6)	0.4212 (4)	0.055 (2)
N1*c*	0.0395 (6)	0.3109 (6)	0.2706 (4)	0.039 (2)
C2*c*	−0.0383 (8)	0.2250 (8)	0.3632 (6)	0.041 (3)
N3*c*	−0.1072 (7)	0.1447 (7)	0.3342 (5)	0.049 (2)
C4*c*	−0.0754 (9)	0.1690 (8)	0.2205 (6)	0.051 (3)
C5*c*	0.0235 (8)	0.2818 (8)	0.1853 (6)	0.039 (2)
N6*c*	−0.0408 (7)	0.2266 (7)	0.4584 (5)	0.055 (2)
C7*c*	−0.1924 (9)	0.0397 (9)	0.4098 (7)	0.072 (4)
O8*c*	0.0812 (6)	0.3370 (5)	0.0940 (4)	0.048 (2)
N1*d*	0.3091 (6)	0.3114 (6)	0.2759 (5)	0.038 (2)
C2*d*	0.3924 (8)	0.2795 (7)	0.1946 (6)	0.039 (3)
N3*d*	0.4741 (7)	0.1858 (7)	0.2168 (5)	0.051 (2)
C4*d*	0.4566 (9)	0.1464 (9)	0.3304 (7)	0.063 (4)
C5*d*	0.3429 (8)	0.2354 (8)	0.3654 (6)	0.044 (3)
N6*d*	0.3926 (7)	0.3380 (7)	0.0954 (5)	0.057 (3)
C7*d*	0.5733 (9)	0.1275 (9)	0.1457 (8)	0.073 (4)
O8*d*	0.2905 (6)	0.2372 (6)	0.4573 (4)	0.062 (2)

Table 2. *Selected geometric parameters (Å, °)*

Pt—N1*a*	2.030 (7)	N3*b*—C4*b*	1.460 (12)
Pt—N1*b*	1.988 (6)	N3*b*—C7*b*	1.432 (11)
Pt—N1*c*	2.034 (7)	C4*b*—C5*b*	1.496 (12)
Pt—N1*d*	1.980 (6)	C5*b*—O8*b*	1.243 (10)
S1—C1	1.595 (11)	N1*c*—C2*c*	1.412 (8)
C1—N1	1.104 (15)	N1*c*—C5*c*	1.330 (11)
S2—C2	1.636 (12)	C2*c*—N3*c*	1.347 (13)
C2—N2	1.115 (15)	C2*c*—N6*c*	1.290 (11)
N1*a*—C2*a*	1.345 (13)	N3*c*—C4*c*	1.441 (10)
N1*a*—C5*a*	1.400 (9)	N3*c*—C7*c*	1.451 (10)
C2*a*—N3*a*	1.332 (11)	C4*c*—C5*c*	1.521 (12)
C2*a*—N6*a*	1.303 (9)	C5*c*—O8*c*	1.220 (8)
N3*a*—C4*a*	1.445 (11)	N1*d*—C2*d*	1.320 (10)
N3*a*—C7*a*	1.453 (15)	N1*d*—C5*d*	1.391 (10)
C4*a*—C5*a*	1.559 (15)	C2*d*—N3*d*	1.310 (11)
C5*a*—O8*a*	1.185 (12)	C2*d*—N6*d*	1.323 (10)
N1*b*—C2*b*	1.395 (12)	N3*d*—C4*d*	1.447 (12)
N1*b*—C5*b*	1.328 (10)	N3*d*—C7*d*	1.452 (12)
C2*b*—N3*b*	1.328 (10)	C4*d*—C5*d*	1.537 (13)
C2*b*—N6*b*	1.304 (10)	C5*d*—O8*d*	1.223 (10)
N1*a*—Pt—N1*b*	89.2 (3)	N3*b*—C4*b*—C5*b*	100.2 (7)
N1*a*—Pt—N1*c*	178.9 (3)	N1*b*—C5*b*—C4*b*	112.7 (7)
N1*a*—Pt—N1*d*	89.9 (3)	N1*b*—C5*b*—O8*b*	123.2 (7)
N1*b*—Pt—N1*c*	91.8 (3)	C4*b*—C5*b*—O8*b*	124.1 (8)
N1*b*—Pt—N1*d*	177.1 (2)	C2*c*—N1*c*—C5*c*	109.6 (7)
N1*c*—Pt—N1*d*	89.1 (3)	N1*c*—C2*c*—N3*c*	108.5 (7)
S1—C1—N1	178.5 (12)	N1*c*—C2*c*—N6*c*	124.2 (8)
S2—C2—N2	179.1 (10)	N3*c*—C2*c*—N6*c*	127.3 (7)
C2*a*—N1*a*—C5*a*	111.8 (7)	C2*c*—N3*c*—C4*c*	111.7 (6)
N1*a*—C2*a*—N3*a*	110.9 (7)	C2*c*—N3*c*—C7*c*	123.1 (7)
N1*a*—C2*a*—N6*a*	122.8 (8)	C4*c*—N3*c*—C7*c*	125.0 (8)
N3*a*—C2*a*—N6*a*	126.3 (10)	N3*c*—C4*c*—C5*c*	101.0 (7)
C2*a*—N3*a*—C4*a*	111.1 (8)	N1*c*—C5*c*—C4*c*	109.2 (6)
C2*a*—N3*a*—C7*a*	125.4 (7)	N1*c*—C5*c*—O8*c*	124.6 (8)
C4*a*—N3*a*—C7*a*	123.5 (7)	C4*c*—C5*c*—O8*c*	126.2 (8)
N3*a*—C4*a*—C5*a*	102.3 (7)	C2*d*—N1*d*—C5*d*	105.4 (6)
N1*a*—C5*a*—C4*a*	103.9 (8)	N1*d*—C2*d*—N3*d*	116.8 (7)
N1*a*—C5*a*—O8*a*	127.2 (9)	N1*d*—C2*d*—N6*d*	121.8 (7)

C4*a*—C5*a*—O8*a*	128.9 (7)	N3*d*—C2*d*—N6*d*	121.4 (7)
C2*b*—N1*b*—C5*b*	105.0 (6)	C2*d*—N3*d*—C4*d*	108.9 (7)
N1*b*—C2*b*—N3*b*	113.3 (7)	C2*d*—N3*d*—C7*d*	129.5 (7)
N1*b*—C2*b*—N6*b*	122.8 (7)	C4*d*—N3*d*—C7*d*	121.6 (7)
N3*b*—C2*b*—N6*b*	123.9 (7)	N3*d*—C4*d*—C5*d*	100.1 (7)
C2*b*—N3*b*—C4*b*	108.7 (7)	N1*d*—C5*d*—C4*d*	108.7 (7)
C2*b*—N3*b*—C7*b*	127.0 (7)	N1*d*—C5*d*—O8*d*	126.1 (8)
C4*b*—N3*b*—C7*b*	122.8 (7)	C4*d*—C5*d*—O8*d*	125.2 (8)

The title structure was solved manually by the Patterson method. H atoms were calculated and refined in a riding geometry with fixed displacement parameters ($U_{\rm iso}$ = 0.0506 Å^2).

Data collection: *CAD*-4 *Manual* (Enraf–Nonius, 1988). Data reduction: *SDP*/*PDP* (Enraf–Nonius, 1985). Program(s) used to refine structure: *SDP*/*PDP*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *KAPPA* (Macíček, 1992).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1187). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Molecular Adducts of Inorganic Salts. VII. $Cd(ReO_4)_2.4tu$ (tu = Thiourea)

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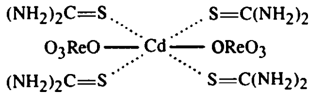
Abstract

The crystal structure of cadmium tetraoxorhenium tetrakis(thiourea), $Cd(ReO_4)_2.4CH_4N_2S$, is comprised of isolated *trans*-[$Cd(ReO_4)_2tu_4$] clusters consisting of a CdS_4O_2 octahedron and two ReO_4 tetrahedra. The Cd—S—C—N torsion angles are −22.6 (5) and 69.1 (4)° for the two thiourea molecules which are inclined at an angle of 10.8 (5)° with respect to one another. The structural units are held together by a complex network of hydrogen bonds.

Comment

The crystal structures of only a few thiourea (tu) addition compounds of cadmium salts are known. These are $CdCl_2.n$tu, with n = 2 (Nardelli, Cavalca & Braibanti, 1957) and n = 4 (Nardelli, Cavalca & Braibanti, 1956), and $CdSO_4.n\text{tu}.mH_2O$, with n = 1 and m = 2 (Cavalca, Domiano, Fava Gasparri & Boldrini, 1967), and n = 3 and m = 0 (Corao & Baggio, 1969; Cavalca, Chiesi Villa, Mangia & Palmieri, 1970). We have investigated the $Cd(ReO_4)_2$–tu–H_2O system and have found several different adducts of formula $Cd(ReO_4)_2.n$tu, where n = 2, 4 and 6. For n = 2, two polymorphic phases have been identified (Petrova, Angelova & Macíček, 1996). One of these phases, (I), is built up of infinite kröhnkite-type chains (Hawthorne & Ferguson, 1975), while in the other, (II), the chains consist of CdS_3O_3 octahedra linked by alternating double ReO_4 and tu bridges.

When n = 4, (1), the structure assumes finite dimensions and consists of isolated centrosymmetric ReO_4–Cd(tu)$_4$–ReO_4 clusters held together by an extensive hydrogen-bonding network. In the notation of Hawthorne (Hawthorne, 1985; Eby & Hawthorne, 1993), this can be represented as *trans*-[$M(T\text{O}_4)_2\varphi_4$]. The same structural unit has been found in $CdCl_2.4$tu (Nardelli, Cavalca & Braibanti, 1956), as well as in the



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