Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances and angles, and inter- and intramolecular distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71356 (35 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL0555]

References

Adams, K. R., Andergg, G., Lindoy, L. F., Lip, H. C., McPartlin, M., Rea, J. H., Smith, R. J. & Tasker, P. A. (1980). *Inorg. Chem.* **19**, 2956–2964.

Adatia, T., McPartlin, M. & Salter, I. D. (1988). *J. Chem. Soc. Dalton Trans.* pp. 751–755.

Ansell, G. B., Modrick, M. A. & Bradley, J. S. (1984). *Acta Cryst.* C**40**, 365–368.

Bateman, L. W., Green, M., Mead, K. A., Stone, F. G. A., Mills, R. M., Salter, I. D. & Woodward, P. (1983). *J. Chem. Soc. Dalton Trans.* pp. 2599–2608.

Bates, P. A., Brown, S. S. D., Dent, A. G., Hursthouse, M. B., Kitchen, G. F. M., Orpen, A. G. & Salter, I. D. (1989). *J. Chem. Soc. Dalton Trans.* pp. 1227–1232.

Blaxill, P., Brown, S. S. D., Frankland, J. C., Salter, I. D. & Sĭk, V. (1989). *J. Chem. Soc. Dalton Trans.* pp. 2039–2047.

Brown, S. S. D., Salter, I. D. & Toupet, L. (1988). *J. Chem. Soc. Dalton Trans.* pp. 757–767.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

Farrugia, L. J., Freeman, M. J., Green, M., Orpen, A. G., Stone, F. G. A. & Salter, I. D. (1983). *J. Organomet. Chem.* **249**, 273–277.

Freeman, M. J., Orpen, A. G. & Salter, I. D. (1987). *J. Chem. Soc. Dalton Trans.* pp. 379–390.

Gabe, E. J., Lee, F. L. & Le Page, Y. (1985). *Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 167–174. Oxford: Clarendon Press.

Orpen, A. G. (1980). *J. Chem. Soc. Dalton Trans.* pp. 2509–2514.

Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination.* Univ. of Cambridge.

Acta Cryst. (1993). C**49**, 1929–1932

Structure of $[Cr_3O(OOCCH_3)_6(OH_2)_3]Cl.3[SC(NH_2)_2].2H_2O$

E. Karu, C. E. Anson, R. D. Cannon,*
U. A. Jayasooriya and A. K. Powell

School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, England

(*Received* 3 *December* 1992; *accepted* 6 *May* 1993)

Abstract

The title compound, hexakis(μ-acetato-κO:$\kappa O'$)-triaqua-1κO,2κO,3κO-μ_3-oxo-trichromium chloride tris(thiourea) dihydrate, has an oxo-centred trinuclear structure with molecular symmetry *m*, the mirror plane relating two of the three Cr atoms, but all three Cr···Cr distances are identical within experimental error [3.289 (1) Å]. The central O atom is within 0.012 Å of the Cr_3 plane. The thiourea molecules are not coordinated but are linked to the coordinated water molecules by hydrogen bonds.

Comment

Oxo-centred trinuclear complexes of the general formula $[M_3O(OOCR)_6L_3]^{n+}$ occur with various trivalent metals, with mixed metals and with mixed valencies, $M_2^{III}M^{II}$. The chemistry and physical properties have been reviewed (Cannon & White, 1988). X-ray and spectroscopic work on compounds of this class has shown that those with three identical metal ions rarely, if ever, show the full $\bar{6}m2$ symmetry of the idealized molecular structure. The prototype salt $[Cr_3O(OOCCH_3)_6(OH_2)_3]Cl.5H_2O$ has the most complicated of all structures, with the trinuclear units on general sites (Figgis & Robertson, 1965; Chang & Jeffrey, 1970), and below a phase-transition temperature of 211 K it has two sets of non-equivalent molecules in each unit cell (Sorai, Tachiki, Suga & Seki, 1971; Schenk & Güdel, 1982; Jayasooriya, Cannon, White & Kearley, 1989). For the interpretation of physical properties it is desirable to find a structure with fewer complications. We report here the structure of a different salt of the same complex cation which has molecular symmetry *m*.

When first reported the title compound was assigned the formula $[Cr_3(OOCCH_3)_6(OH)_2(H_2NCSNH_2)_3]Cl.xH_2O$, with $x = 2$ or 3 (Weinland & Hachenburg, 1923). In view of the later work on complexes of this type, cited above, this could be revised to the oxo-centred form, and by analogy with other known structures the three thiourea molecules could be expected to be bonded to the three Cr atoms, as $[Cr_3(OOCCH_3)_6O(H_2NCSNH_2)_3]Cl.(x+1)H_2O$. However, all our attempts to detect inner-sphere coordination of thiourea were unsuccessful. Visible–UV spectra and kinetic behaviour in solution, and IR and Raman spectra of the solid, suggested the tris(aqua) formulation; this is now confirmed.

The structure is remarkable for the regularity of the central Cr atom triangle. Two Cr atoms are related by the mirror plane of symmetry which passes through the third, and all three Cr···Cr distances are identical within experimental error [3.289 (1) Å]. The three central O—Cr distances differ by only 0.005 Å [1.902 (3) and 1.897 (1) Å] and the central O atom is within 0.012 Å of the Cr_3 plane. This is a very small displacement and probably not significant when compared with the probable positional e.s.d. of *ca* 0.004 Å. As shown in Fig. 2, each terminal H_2O molecule is hydrogen bonded

Acta Crystallographica Section C
ISSN 0108-2701 © 1993

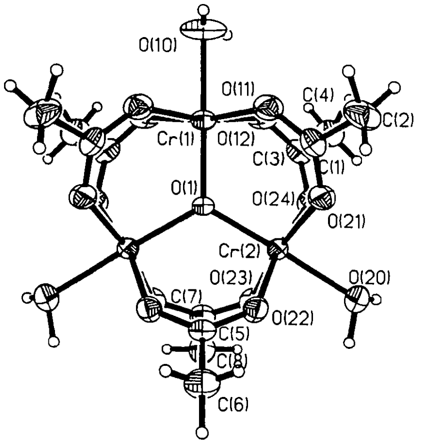

Fig. 1. Structure of the complex ion in $[Cr_3O(OOCCH_3)_6(OH_2)_3]Cl.3[SC(NH_2)_2].2H_2O$.

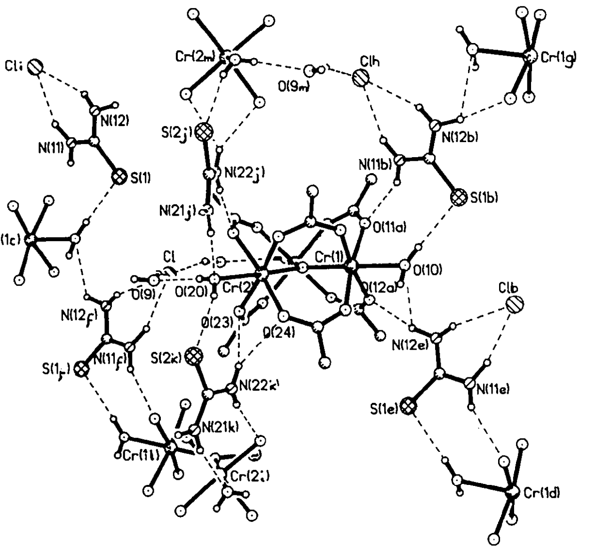

Fig. 2. Hydrogen bonding in the crystal structure of the title compound.

to two thiourea molecules, and each thiourea is hydrogen bonded to two complex molecules. One of the H atoms is involved in an almost symmetrically bifurcated bond, from N(22) to O(23) and O(24).

Our interest in these materials is mainly to do with their magneto-optic properties arising from the intra- and intermolecular electronic interactions of the metal atoms (Cannon, Jayasooriya & White, 1991). From this point of view, the present compound is a promising test substance, since not only are the complex ions close to ideal geometry, they are also conveniently aligned in the crystal. As shown in Figs. 2 and 3, the molecules are stacked in columns and all the Cr_3 planes are inclined at ±6.1° to the {100} plane of the crystal.

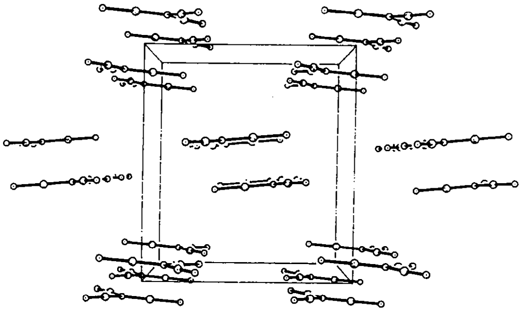

Fig. 3. Perspective view of the crystal structure of the title compound along the *b* axis, showing the inclination of the $O(CrO)_3$ units to the {100} plane.

Experimental

Crystal data

$[Cr_3O(C_2H_3O_2)_6(H_2O)_3]Cl.3(CH_4N_2S).2H_2O$
$M_r = 880.13$
Orthorhombic
Pnma
$a = 15.156\ (2)$ Å
$b = 17.340\ (3)$ Å
$c = 13.472\ (2)$ Å
$V = 3540.4\ (8)$ Å^3
$Z = 4$
$D_x = 1.65$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 3.1$-$12.9°$
$\mu = 1.20$ mm^{-1}
$T = 295$ K
Block
0.42 × 0.30 × 0.26 mm
Dark green

Data collection

Nicolet-Siemens *P*3/*V* diffractometer
ω scans
Absorption correction: spherical (ψ scan)
$T_{min} = 0.225$, $T_{max} = 0.265$
8705 measured reflections
4209 independent reflections
3482 observed reflections $[F_o \geq 5\sigma(F_o)]$

$R_{int} = 0.0205$
$\theta_{max} = 22.5°$
$h = -18 \rightarrow 18$
$k = 0 \rightarrow 20$
$l = 0 \rightarrow 23$
2 standard reflections monitored every 50 reflections intensity variation: not significant

Refinement

Refinement on *F*
Final $R = 0.0513$
$wR = 0.0447$
$S = 2.62$
3482 reflections
286 parameters
$w = 1/[\sigma^2(F) + 0.00005F^2]$

$(\Delta/\sigma)_{max} = 0.504$ [for *y* of H(42)]
$\Delta\rho_{max} = 0.481$ e Å^{-3}
$\Delta\rho_{min} = -0.524$ e Å^{-3}
Atomic scattering factors from Cromer & Waber (1974)

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

$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$

	x	*y*	*z*	U_{eq}
Cr(1)	0.10341 (5)	0.2500	−0.01669 (5)	0.0255
Cr(2)	0.08348 (3)	0.15517 (3)	0.19352 (3)	0.0227
O(1)	0.0909 (2)	0.2500	0.1238 (2)	0.0226
O(10)	0.1152 (2)	0.2500	−0.1673 (2)	0.0527

O(11)	0.1970 (2)	0.1714 (1)	−0.0191 (2)	0.0372
O(12)	0.0113 (2)	0.1722 (1)	−0.0384 (2)	0.0413
O(20)	0.0788 (2)	0.0536 (2)	0.2740 (2)	0.0362
O(21)	0.1808 (1)	0.1047 (1)	0.1215 (2)	0.0359
O(22)	0.1700 (1)	0.1855 (1)	0.2959 (2)	0.0324
O(23)	−0.0188 (1)	0.1857 (1)	0.2741 (2)	0.0344
O(24)	−0.0034 (1)	0.1079 (1)	0.1039 (2)	0.0372
C(1)	0.2185 (2)	0.1182 (2)	0.0392 (2)	0.0316
C(2)	0.2928 (3)	0.0665 (3)	0.0103 (3)	0.0489
C(3)	−0.0239 (2)	0.1220 (2)	0.0141 (2)	0.0315
C(4)	−0.0948 (3)	0.0736 (2)	−0.0311 (3)	0.0465
C(5)	0.1953 (3)	0.2500	0.3291 (3)	0.0302
C(6)	0.2618 (4)	0.2500	0.4113 (4)	0.0499
C(7)	−0.0509 (3)	0.2500	0.2971 (3)	0.0304
C(8)	−0.1350 (4)	0.2500	0.3548 (4)	0.0417
Cl	0.0441 (1)	0.2500	0.5303 (1)	0.0700
O(9)	0.0588 (4)	0.0795 (2)	0.4672 (3)	0.1083
S(1)	0.2799 (1)	0.2500	0.6900 (1)	0.0452
C(11)	0.3656 (3)	0.2500	0.7730 (4)	0.0404
N(11)	0.3563 (4)	0.2744 (5)	0.8649 (4)	0.0687
N(12)	0.4426 (4)	0.2185 (4)	0.7488 (5)	0.0616
S(2)	0.0782 (1)	0.4345 (1)	0.7407 (1)	0.0549
C(21)	0.1744 (2)	0.4836 (2)	0.7528 (3)	0.0392
N(21)	0.2513 (2)	0.4495 (2)	0.7371 (3)	0.0779
N(22)	0.1756 (2)	0.5573 (2)	0.7784 (3)	0.0513

Table 2. *Geometric parameters* (Å, °)

Primed atoms are generated by the symmetry operation (x, $\frac{1}{2} - y$, z).

Cr(1)—Cr(2)	3.289 (1)	Cr(2)—Cr(2)′	3.289 (1)
Cr(1)—O(1)	1.902 (3)	Cr(2)—O(1)	1.897 (1)
Cr(1)—O(10)	2.037 (3)	Cr(2)—O(20)	2.070 (3)
Cr(1)—O(11)	1.968 (2)	Cr(1)—O(12)	1.963 (2)
Cr(2)—O(21)	1.970 (2)	Cr(2)—O(22)	1.974 (2)
Cr(2)—O(23)	1.965 (2)	Cr(2)—O(24)	1.966 (2)
C(1)—O(11)	1.255 (4)	C(1)—O(21)	1.269 (4)
C(3)—O(12)	1.242 (4)	C(3)—O(24)	1.272 (4)
C(5)—O(22)	1.264 (3)	C(7)—O(23)	1.254 (3)
C(1)—C(2)	1.492 (5)	C(3)—C(4)	1.493 (5)
C(5)—C(6)	1.498 (6)	C(7)—C(8)	1.493 (7)
S(1)—C(11)	1.715 (6)	S(2)—C(21)	1.696 (4)
C(11)—N(11)	1.315 (8)	C(21)—N(21)	1.324 (5)
C(11)—N(12)	1.328 (7)	C(21)—N(22)	1.323 (5)
Cr(1)—O(1)—Cr(2)	119.9 (1)	Cr(2)—O(1)—Cr(2)′	120.2 (1)
O(1)—Cr(1)—O(10)	179.3 (1)	O(1)—Cr(2)—O(20)	177.6 (1)
O(1)—Cr(1)—O(11)	95.1 (1)	O(10)—Cr(1)—O(11)	85.4 (1)
O(1)—Cr(1)—O(12)	94.4 (1)	O(10)—Cr(1)—O(12)	85.1 (1)
O(1)—Cr(2)—O(21)	95.6 (1)	O(20)—Cr(2)—O(21)	84.6 (1)
O(1)—Cr(2)—O(22)	94.3 (1)	O(20)—Cr(2)—O(22)	83.3 (1)
O(1)—Cr(2)—O(23)	95.0 (1)	O(20)—Cr(2)—O(23)	85.0 (1)
O(1)—Cr(2)—O(24)	95.6 (1)	O(20)—Cr(2)—O(24)	86.8 (1)
O(11)—Cr(1)—O(12)	92.0 (1)	O(11)—Cr(1)—O(11)′	87.7 (2)
O(12)—Cr(1)—O(12)′	86.8 (2)	O(21)—Cr(2)—O(22)	88.0 (1)
O(22)—Cr(2)—O(23)	93.8 (1)	O(23)—Cr(2)—O(24)	85.6 (1)
O(21)—Cr(2)—O(24)	90.8 (1)	O(21)—Cr(2)—O(23)	169.2 (1)
O(22)—Cr(2)—O(24)	170.1 (1)	Cr(1)—O(12)—C(3)	134.6 (2)
Cr(1)—O(11)—C(1)	133.3 (2)	Cr(2)—O(22)—C(5)	133.2 (2)
Cr(2)—O(21)—C(1)	133.3 (2)	Cr(2)—O(24)—C(3)	131.9 (2)
Cr(2)—O(23)—C(7)	133.0 (2)	O(12)—C(3)—O(24)	124.8 (3)
O(11)—C(1)—O(12)	124.5 (3)	O(23)—C(7)—O(23)	125.3 (4)
O(22)—C(5)—O(22)′	124.4 (4)	S(2)—C(21)—N(21)	121.3 (3)
S(1)—C(11)—N(12)	120.4 (4)	S(2)—C(21)—N(22)	121.4 (3)
N(11)—C(11)—N(12)	117.2 (6)	N(21)—C(21)—N(22)	117.4 (4)
O(10)···N(12^{i})	2.889	Cl···N(11^{v})	3.205
O(20)···N(21^{ii})	3.184	Cl···N(12^{v})	3.393
O(11)···N(11^{iii})	3.026	O(9)···O(20)	2.659
O(12)···N(12^{i})	3.125	S(1^{vi})···O(10)	3.150
O(24)···N(22^{iv})	3.181	S(2^{iv})···O(20)	3.156
Cl···O(9)	3.084	O(23)···N(22^{iv})	3.333

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z$; (ii) $\frac{1}{2} - x, y - \frac{1}{2}, z - \frac{1}{2}$; (iii) $x, \frac{1}{2} - y, z - 1$; (iv) $-x, y - \frac{1}{2}, 1 - z$; (v) $x - \frac{1}{2}, \frac{1}{2} - y, \frac{3}{2} - z$.

Chromium trioxide was finely ground and dried over P_2O_5 for a few hours. Anhydrous AnalaR acetic acid and thiourea were used without further purification. Chromium trioxide (5.1 g, 0.051 mol) was heated under reflux with acetic acid (12 g, 0.2 mol) on a steam bath with stirring. Ethanol was added dropwize with constant stirring, the vigorous reaction being allowed to subside fully after each drop before adding the next. A total of 15 ml of ethanol was used over a period of *ca* 90 min before finally a thick pure green solution remained. Thiourea (3.9 g, 0.050 mol) was added and heating and stirring were continued under reflux on a steam bath for 1 h. Concentrated aqueous HCl (4 ml) was added slowly with stirring and heating was continued for 10 min. The filtrate was allowed to cool in open air. After 24-48 h, shiny green crystals were filtered off, washed with ether and dried in air. Yield 6.4 g. Further evaporation of the filtrate gave a further 2.8 g of product. Elemental analysis: calculated for $C_{15}H_{40}ClCr_3N_3O_{17}S_3$ C 20.42, H 4.54, Cl 4.03, N 9.53, S 10.89%; found C 20.47, H 4.51, Cl 4.08, N 9.21, S 10.49%. Thiourea was also determined spectrophotometrically using the yellow colour developed on reaction with *p*-dimethylaminobenzaldehyde in aqueous ethanol acidified with 0.4 *M* HCl. In two determinations, the thiourea/trinuclear complex ratio was obtained as 3.01 and 3.02.

Systematic absences indicated possible space groups *Pna*2_1 or *Pnma* and the structure was successfully solved in the latter. The Cr atoms were located from a Patterson synthesis. The remaining non-H atoms were located from successive least-squares refinements and difference Fourier maps. It was found that one of the thiourea molecules was situated on a mirror plane, the C—S bond lying in the plane, but the N atoms were disordered above and below the plane and were refined as two pairs of half atoms. Further cycles of refinement and difference Fourier maps located all the H atoms. An H atom in one of the aqua ligands was also disordered on either side of the mirror plane. All methyl C—H distances were constrained to 0.96 (1) Å and the bond distance O(10)—H(101) was constrained to 0.85 (2) Å. The H(102), H(111), H(112), H(121) and H(122) atoms were located but their positions were not refined. Positional parameters of all other H atoms were refined freely. All H atoms were assigned isotropic thermal parameters $U = 1.2 \times U_{\rm iso}$, where the values of $U_{\rm iso}$ relate to the atoms to which the H atoms are bonded. All non-H atoms were then assigned anisotropic temperature factors. The function minimized was $\Sigma(w|\Delta F|^2)$.

This work was supported by the Science and Engineering Research Council and the Bauchi State Government (Nigeria).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and bond distances and angles including H-atom geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71308 (32 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL1037]

References

Cannon, R. D., Jayasooriya, U. A. & White, R. P. (1991). *Mixed Valency Systems: Applications in Chemistry, Physics and Biology*, edited by K. Prassides. *NATO ASI Series C: Mathematical and Physical Sciences*, Vol. 343, pp. 283-298. Dordrecht: Kluwer Academic Publishers.

Cannon, R. D. & White, R. P. (1988). *Prog. Inorg. Chem.* **36**, 195–298.
Chang, S. C. & Jeffrey, G. A. (1970). *Acta Cryst.* B**26**, 673–683.
Cromer, D. T. & Waber, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Table 2.2A, pp. 149–150. Birmingham: Kynock Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
Figgis, B. N. & Robertson, G. B. (1965). *Nature* (*London*), **205**, 694.
Jayasooriya, U. A., Cannon, R. D., White, R. P. & Kearley, G. J. (1989). *Angew. Chem. Int. Ed. Engl.* **28**, 930–931.
Schenk, K. J. & Güdel, H. U. (1982). *Inorg. Chem.* **21**, 2253–2256.
Sorai, M., Tachiki, M., Suga, H. & Seki, S. (1971). *J. Phys. Soc. Jpn*, **30**, 750–759.
Weinland, R. & Hachenburg, H. (1923). *Z. Anorg. Chem.* **126**, 285–304.

Acta Cryst. (1993). C**49**, 1932–1934

Structure of (Pyrazole-κN^2)[(*S*)-*N*-salicylidene-κO-alaninato(2−)-κN,κO]copper(II)–Pyrazole (1/1)

Viktor Kettmann* and Eva Frešová

Department of Analytical Chemistry, Faculty of Pharmacy, Comenius University, Odbojárov 10, 83232 *Bratislava, Czechoslovakia*

Mária Bláhová and Juraj Krätsmár-Šmogrovič

Department of Inorganic Chemistry, Faculty of Pharmacy, Comenius University, Odbojárov 10, 83232 *Bratislava, Czechoslovakia*

(*Received* 14 *December* 1992; *accepted* 7 *April* 1993)

Abstract

Reaction of the parent aqua[(*S*)-*N*-salicylidene-alaninato]copper(II) dihydrate with an excess of pyrazole gives the title compound in which only one of the two pyrazole molecules is coordinated to Cu^{II} (the other is doubly hydrogen bonded to the complex molecule). The Cu^{II} coordination can be described as square pyramidal (4 + 1), the basal plane being formed by the heteroatoms of the tridentate Schiff base ligand and the N atom of the pyrazole molecule. A neighbouring chelate provides a semi-coordinating O(3) atom in the axial direction [Cu⋯O(3) = 2.595 (3) Å], thus forming polymeric chains along the *a* axis in the crystal. The title complex serves as a model to study the mechanism of a racemization reaction of amino acids catalyzed by vitamin B_6 (or salicylaldehyde) and metal ions. The results, combined with those obtained previously for potassium isocyanato[(*R*,*S*)-*N*-salicylidene-alaninato]cuprate(II), do not support the general mechanism proposed earlier for the racemization reaction but instead suggest an active role for the nucleophilic solvent in the catalytic reaction.

Comment

This work is part of a more general study on the structural and chemical properties of copper complexes of Schiff bases derived from salicylaldehyde and amino acids. These complexes attract much attention owing to their biological importance since they serve as models for the more complicated key intermediates in the enzymatically catalyzed metabolic reactions of amino acids (Guirard & Snell, 1964; Bkouche-Waksman, Barbe & Kvick, 1988, and references therein). Recently, we reported (Krätsmár-Šmogrovič, Bláhová & Kettmann, 1991; Kettmann, Krätsmár-Šmogrovič & Švajlenová, 1990) that treatment of [Cu({sal-(*S*)-Ala}(H_2O)].2H_2O [sal-(*S*)-Ala = *N*-salicylidene-(*S*)-alaninato] with an excess of KOCN in hot dilute methanol led to a racemic product of composition K[Cu({sal-(*RS*)-Ala}(NCO))] (I). Although the title compound (II) was prepared under identical conditions, except for using pyrazole in place of KOCN, the racemization of the Schiff base ligand was not observed. To obtain a structural basis for understanding this difference in kinetic behaviour between (I) and (II), an X-ray analysis of (II) was undertaken.

The title complex was prepared by treatment of 3.1 g (10 mmol) of [Cu{sal-(*S*)-Ala}(H_2O)].2H_2O with 2.7 g (40 mmol) of pyrazole in dilute (65%) methanol at 233 K. After filtration and slow cooling to room temperature, dark-green single crystals appeared.

The numbering scheme is shown in Fig. 1, which also displays the overall conformation of the molecule and corresponds to the correct *S* enantiomer.

As generally found for this type of complex, the coordination geometry around Cu^{II} is axially distorted square pyramidal (4 + 1), the four basal atoms being O(1), N(1) and O(2) of the Schiff base ligand and the N(2) atom of one of the pyrazole molecules. The second, uncoordinated, pyrazole molecule associates with the complex through two hydrogen bonds. A neighbouring chelate provides the semi-coordinating O(3) atom in the axial direction [Cu⋯O(3)($x - 1$, y, z) = 2.595 (3) Å] to complete the coordination. There is another contact shorter than the sum of the van der Waals radii, namely N(3)⋯O(2), so that the H atom on N(3) may be regarded as being involved in a bifurcated hydrogen bond.

The mean plane through the four basal atoms shows a slight tetrahedral distortion from planarity and the Cu atom is displaced from this plane by 0.145 (1) Å toward the apex of the pyramid. The