

held together by the Cl^- ions. The structure determination shows that the range of interaction extends only to next-nearest neighbours. The more bulky ClO_4^- ions in the ordered structure lead to an entirely different hydrogen-bonded structure. O(11) and O(2) both accept two hydrogen bonds each, with $\text{O}\cdots\text{H}-\text{N}$ angles between 161 and 166° , whereas O(3) has a close contact of 2.46 \AA with H(1), the angle $\text{C}(2)-\text{H}(1)\cdots\text{O}(3)$ being 142° .

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References

- CREITZ, T. C., GSELL, R. & WAMPLER, D. L. (1969). *Chem. Commun.* pp. 1371–1372.
- CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.
- CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* **A24**, 321–324.
- DORNBERGER-SCHIFF, K. (1966). *Lehrgang über OD Strukturen*. Berlin: Akademie-Verlag.
- ERNST, R. (1977). *Acta Cryst.* **B33**, 237–240.
- ERNST, R. & CAGLE, F. W. (1977). *Acta Cryst.* **B33**, 235–237.
- HOLIAN, B. L. & MARSH, R. E. (1970). *Acta Cryst.* **B26**, 1049–1058.
- JAGDZINSKI, H. (1949). *Acta Cryst.* **2**, 201–207.
- LEWIS, R. M., NANCOLLAS, G. H. & COPPENS, P. (1972). *Inorg. Chem.* **11**, 1371–1375.
- LIS, T., MATUSZEWSKI, J. & JEŻOWSKA-TRZEBIATOWSKA, B. (1977). *Acta Cryst.* **B33**, 1943–1946.
- MATHEW, M. & KUNCHUR, N. R. (1970). *Acta Cryst.* **B26**, 2054–2062.
- MÉRING, J. (1949). *Acta Cryst.* **2**, 371–377.
- NIGGLI, A. (1964). *Adv. Struct. Res. Diffr. Methods*, **1**, 199–221.
- PINKERTON, A. A. & SCHWARZENBACH, D. (1977). Collect. Abstr. 4th Eur. Crystallogr. Meet. PII.126.
- SCHWARZENBACH, D. (1969). *Z. Kristallogr.* **128**, 97–114.
- SCHWARZENBACH, D. (1977). Collect. Abstr. 4th Eur. Crystallogr. Meet. PI.20.
- SCHWARZENBACH, G. & SCHWARZENBACH, D. (1977). *J. Indian Chem. Soc.* **54**, 23–24.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.
- XRAY system (1972). Tech. Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland. Implemented and extended by D. SCHWARZENBACH.
- ZACHARIASEN, W. H. (1967). *Acta Cryst.* **23**, 558–564.

Acta Cryst. (1978). **B34**, 1833–1837

The Crystal and Molecular Structure of Tetrachloroqua[2,4,6-tris(2'-pyridyl)-1,3,5-triazine]dicobalt(II) Monohydrate

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$[\text{C}_{18}\text{H}_{12}\text{N}_6(\text{H}_2\text{O})\text{Co}_2\text{Cl}_4] \cdot \text{H}_2\text{O}$ is monoclinic, space group $P2_1/a$, with $a = 26.77(7)$, $b = 10.88(3)$, $c = 8.63(2) \text{ \AA}$, $\beta = 99.2(2)^\circ$, $Z = 4$. The structure was refined to $R = 0.108$ for 708 visually estimated reflexions. The ligand functions primarily as tridentate and monodentate to the two Co atoms. Co(1) is at the centre of a distorted octahedron of two Cl atoms [Co–Cl $2.23(1)$, $2.55(1) \text{ \AA}$], one water molecule [Co–O $2.19(3) \text{ \AA}$] and three N atoms of the ligand [mean Co–N $2.07(3) \text{ \AA}$]. Co(2) is surrounded by three Cl atoms [mean Co–Cl $2.22(1) \text{ \AA}$] and one pyridyl N atom [Co–N $1.99(3) \text{ \AA}$] forming a distorted tetrahedron. A Cl atom bridges Co(1) and Co(2) of adjacent molecules to form molecular chains parallel to [010]. Severe distortions in the ligand molecule are apparent. The uncoordinated water molecule is associated with the coordinated water, two Cl atoms and the s-triazine ring, which shows distortion to a chair conformation.

Introduction

2,4,6-Tris(2'-pyridyl)-1,3,5-triazine (tpt) has been shown to function primarily as a tridentate ligand with a variety of transition-metal salts (Barclay, Vagg & Watton, 1977a). From non-aqueous media dimeric

species of general formula $M_2X_4\text{tpt} \cdot n\text{H}_2\text{O}$ (where $M = \text{Ni}$ or Co ; $X = \text{Cl}$ or Br) have been isolated where the ligand may be acting simultaneously as both tridentate and bidentate (Vagg, Warrener & Watton, 1967, 1969). We have reported the crystal structures of a bivalent Ni complex (Barclay, Vagg & Watton, 1977a)

and a pentachloromanganate salt (Barclay, Vagg & Watton, 1977b) of tpt. We report here the structure of $\text{Co}_2\text{Cl}_4\text{tpt} \cdot 2\text{H}_2\text{O}$.

Experimental

The complex was obtained as dark-green plates from the reaction of tpt with excess $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ in hot ethanol/acetone. The product was found to be very unstable, absorbing moisture from the atmosphere in a short time and changing to orange/red with simultaneous loss of crystalline properties. Mounted unprotected on a goniometer head the crystals showed decomposition within 30 min, which could not be arrested by Lindemann-glass capillaries or by a lacquer coating. However, when sealed under a dry gelatin capsule in the presence of several other crystals and one or two pieces of silica gel the compound remains stable for several hours.

Crystal data

$\text{C}_{18}\text{H}_{16}\text{N}_6\text{O}_2\text{Cl}_4\text{Co}_2$, $M_r = 608.0$, monoclinic, $a = 26.77$ (7), $b = 10.88$ (3), $c = 8.63$ (2) Å, $\beta = 99.2$ (2)°, $U = 2481.2$ Å³, $D_m = 1.61$ (by flotation), $D_c = 1.628$ g cm⁻³, $F(000) = 1216$, $\mu(\text{Cu } K\alpha) = 15.0$ cm⁻¹. Systematic absences: $0k0$ when $k = 2n + 1$, $h0l$ when $h = 2n + 1$; space group $P2_1/a$.

Cell parameters were determined with several crystals from rotation photographs with unfiltered Cu radiation. One crystal only, $0.05 \times 0.5 \times 0.2$ mm, mounted as described above about $[010]$, was found to be stable for 8–9 days before significant decomposition occurred. During this period 708 non-zero reflexions were recorded on layers $h0-6l$ by the equi-inclination Weissenberg method with unfiltered Cu radiation. Intensities were measured visually. They were corrected for Lorentz-polarization and absorption (Coppens, Leiserowitz & Rabinovich, 1965) effects but not for extinction, and initially were scaled according to exposure time.

Scattering factors were taken from *International Tables for X-ray Crystallography* (1962). Initial refinement was carried out on an IBM 360/50 computer with *ORFLS* (Busing, Martin & Levy, 1962), and later on a Univac 1106 computer with programs written by F. S. Stephens.

Structure determination

The structure was solved by the heavy-atom method. Isotropic refinement was by full-matrix least-squares calculations, in which the function minimized was $\sum w\Delta^2$, and with unit weights. Initially an overall scale factor and positional and individual isotropic thermal

parameters were varied; in the latter stages of isotropic refinement a scale factor for each level was varied.

H atom positions were calculated for the three pyridyl rings but were not refined. Finally, anisotropic thermal parameters were used for the Co and Cl atoms together with an overall scale factor and a weighting scheme, $w = (62.5 - 0.10|F_o| + 0.013|F_o|^2)^{-1}$. Reflexions for which $|F_c| < 0.33|F_o|$ were omitted from the refinement, which was terminated when the maximum shift in any parameter was $< 0.1\sigma$. 704 reflexions were included in the final cycle. A final difference synthesis showed maximum positive electron densities of $0.9 \text{ e } \text{Å}^{-3}$ near the heavy atoms. The final R

Table 1. Final atomic coordinates (fractional, $\times 10^3$) and isotropic thermal parameters (Å²) with estimated standard deviations in parentheses

For all H atoms $B = 5.0 \text{ Å}^2$.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>
Co(1)	396.6 (3)	331.4 (7)	175.9 (8)	
Co(2)	176.7 (2)	489.0 (7)	-206.6 (8)	
Cl(11)	478.7 (4)	285.2 (12)	194.7 (15)	
Cl(12)	381.4 (4)	128.4 (11)	308.2 (13)	
Cl(21)	244.8 (4)	596.9 (11)	-217.8 (14)	
Cl(22)	162.9 (4)	318.5 (11)	-351.5 (14)	
O(1)	407 (1)	512 (3)	74 (3)	4.1 (8)
O(2)	325 (1)	638 (3)	72 (4)	5.3 (9)
N(1)	322 (1)	373 (4)	154 (4)	3.2 (9)
N(2)	259 (2)	436 (4)	271 (4)	3.5 (9)
N(3)	246 (1)	370 (3)	11 (4)	1.7 (8)
N(11)	364 (1)	274 (3)	-46 (4)	1.6 (8)
N(21)	386 (1)	419 (3)	388 (4)	1.8 (8)
N(31)	150 (1)	444 (3)	-11 (3)	1.6 (8)
C(1)	293 (2)	346 (4)	25 (6)	4.0 (12)
C(2)	306 (2)	414 (5)	279 (6)	4.1 (13)
C(3)	230 (2)	396 (4)	134 (5)	2.6 (11)
C(11)	318 (2)	289 (5)	-96 (6)	4.7 (13)
C(12)	290 (2)	250 (4)	-242 (5)	3.4 (12)
C(13)	320 (2)	208 (5)	-344 (5)	4.5 (13)
C(14)	371 (2)	180 (4)	-307 (5)	3.0 (12)
C(15)	386 (2)	224 (4)	-154 (5)	3.1 (11)
C(21)	342 (2)	451 (4)	418 (5)	2.9 (11)
C(22)	329 (2)	503 (4)	539 (5)	2.5 (11)
C(23)	366 (2)	538 (4)	668 (6)	4.2 (12)
C(24)	411 (2)	511 (5)	637 (6)	4.5 (12)
C(25)	420 (2)	462 (4)	507 (5)	2.9 (11)
C(31)	178 (2)	413 (4)	130 (5)	1.3 (9)
C(32)	160 (2)	381 (4)	260 (5)	1.8 (9)
C(33)	110 (2)	373 (4)	244 (5)	3.5 (12)
C(34)	79 (2)	405 (4)	109 (5)	3.1 (12)
C(35)	102 (2)	445 (5)	-14 (6)	4.2 (12)
H(12)	253	244	-268	
H(13)	310	194	-460	
H(14)	397	148	-369	
H(15)	418	218	-68	
H(22)	292	504	537	
H(23)	360	580	765	
H(24)	444	516	714	
H(25)	456	469	483	
H(32)	184	373	369	
H(33)	91	338	326	
H(34)	42	404	89	
H(35)	83	469	-113	

based on all 708 reflexions was 0.108 and R' $[= (\sum w\Delta^2 / \sum w|F_o|^2)^{1/2}]$ was 0.138. Atomic coordinates and isotropic thermal parameters for the lighter atoms are given in Table 1.*

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33303 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. Bond lengths (Å) and angles (°) with estimated standard deviations in parentheses

Co(1)—Cl(11)	2.23 (1)	Co(1)—Cl(12)	2.55 (1)
Co(1)—O(1)	2.19 (3)	Co(1)—N(11)	2.07 (3)
Co(1)—N(1)	2.03 (4)	Co(1)—N(21)	2.12 (3)
Co(2)—Cl(12 ¹)	2.25 (1)	Co(2)—Cl(21)	2.19 (1)
Co(2)—Cl(22)	2.23 (1)	Co(2)—N(31)	1.99 (3)
N(1)—C(1)	1.29 (5)	N(1)—C(2)	1.29 (5)
C(2)—N(2)	1.28 (5)	N(2)—C(3)	1.38 (4)
C(3)—N(3)	1.24 (5)	N(3)—C(1)	1.27 (5)
N(11)—C(11)	1.26 (5)	C(11)—C(12)	1.42 (6)
C(12)—C(13)	1.38 (6)	C(13)—C(14)	1.38 (5)
C(14)—C(15)	1.40 (5)	C(15)—N(11)	1.29 (5)
N(21)—C(21)	1.31 (5)	C(21)—C(22)	1.28 (5)
C(22)—C(23)	1.42 (5)	C(23)—C(24)	1.32 (6)
C(24)—C(25)	1.30 (5)	C(25)—N(21)	1.34 (4)
N(31)—C(31)	1.36 (4)	C(31)—C(32)	1.33 (5)
C(32)—C(33)	1.35 (5)	C(33)—C(34)	1.37 (5)
C(34)—C(35)	1.38 (6)	C(35)—N(31)	1.30 (5)
C(1)—C(11)	1.46 (6)	C(2)—C(21)	1.47 (5)
C(3)—C(31)	1.41 (5)		

Discussion

Bond distances and angles are given in Table 2. Fig. 1 shows a perspective drawing of the molecule and the labelling of the atoms (Johnson, 1965). Fig. 2 shows the packing viewed down c .

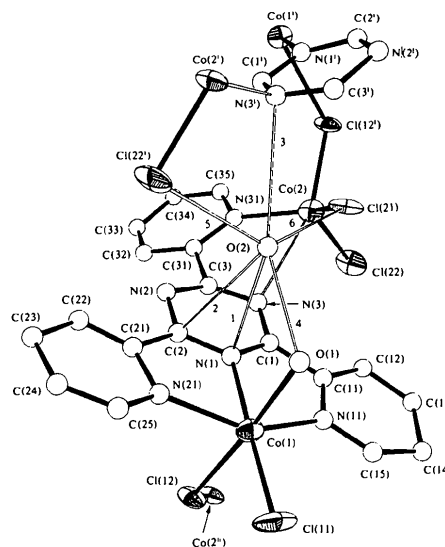


Fig. 1. Perspective drawing of the molecule showing the labelling of the atoms. Intermolecular contacts to O(2) are shown and are numbered according to details given in Table 4. Anisotropic thermal ellipsoids are scaled to include 35% probability.

Table 2 (cont.)

Cl(11)—Co(1)—Cl(12)	89.9 (5)	O(1)—Co(1)—N(11)	87.6 (13)	Cl(12)—Co(1)—N(21)	87.2 (10)
Cl(11)—Co(1)—N(11)	105.0 (12)	O(1)—Co(1)—N(21)	89.2 (13)	N(1)—Co(1)—N(11)	74.1 (16)
Cl(11)—Co(1)—N(21)	107.3 (13)	Cl(12)—Co(1)—O(1)	176.2 (9)	N(1)—Co(1)—N(21)	73.6 (16)
Cl(11)—Co(1)—N(1)	179.0 (12)	Cl(12)—Co(1)—N(1)	90.6 (12)	N(11)—Co(1)—N(21)	147.7 (14)
Cl(11)—Co(1)—O(1)	92.4 (9)	Cl(12)—Co(1)—N(11)	94.7 (10)	Co(1)—Cl(12)—Co(2 ^b)	124.1 (4)
O(1)—Co(1)—N(1)	87.1 (14)				
Cl(21)—Co(2)—Cl(22)	119.0 (4)	Cl(22)—Co(2)—N(31)	102.9 (5)	Cl(22)—Co(2)—Cl(12 ¹)	107.5 (4)
Cl(21)—Co(2)—N(31)	125.4 (3)	Cl(21)—Co(2)—Cl(12 ¹)	98.6 (1)	Cl(12 ¹)—Co(2)—N(31)	100.5 (3)
Co(1)—N(1)—C(1)	118 (4)	Co(1)—N(1)—C(2)	117 (4)	Co(2)—N(31)—C(31)	127 (2)
Co(1)—N(11)—C(11)	121 (4)	Co(1)—N(11)—C(15)	129 (3)	Co(2)—N(31)—C(35)	118 (3)
Co(1)—N(21)—C(21)	123 (3)	Co(1)—N(21)—C(25)	131 (3)		
C(1)—N(1)—C(2)	125 (5)	C(21)—N(21)—C(25)	106 (4)	C(1)—C(11)—C(12)	121 (6)
C(2)—N(2)—C(3)	113 (5)	C(21)—C(22)—C(23)	120 (5)	C(2)—C(21)—C(22)	124 (5)
C(3)—N(3)—C(1)	116 (5)	C(23)—C(24)—C(25)	124 (5)	C(3)—C(31)—C(32)	115 (4)
C(11)—C(1)—N(1)	117 (6)	C(31)—N(31)—C(35)	115 (4)	N(11)—C(11)—C(12)	128 (6)
C(21)—C(2)—N(1)	122 (6)	C(31)—C(32)—C(33)	115 (4)	C(12)—C(13)—C(14)	126 (5)
C(31)—C(3)—N(2)	113 (4)	C(33)—C(34)—C(35)	117 (5)	C(14)—C(15)—N(11)	137 (5)
C(1)—C(11)—N(11)	110 (5)	N(1)—C(2)—N(2)	118 (5)	N(21)—C(21)—C(22)	131 (5)
C(2)—C(21)—N(21)	104 (5)	N(2)—C(3)—N(3)	126 (5)	C(22)—C(23)—C(24)	110 (5)
C(3)—C(31)—N(31)	116 (4)	N(3)—C(1)—N(1)	118 (5)	C(24)—C(25)—N(21)	129 (5)
C(11)—N(11)—C(15)	110 (5)	C(11)—C(1)—N(3)	125 (6)	N(31)—C(31)—C(32)	127 (4)
C(11)—C(12)—C(13)	112 (5)	C(21)—C(2)—N(2)	119 (6)	C(32)—C(33)—C(34)	122 (5)
C(13)—C(14)—C(15)	105 (4)	C(31)—C(3)—N(3)	119 (5)	C(34)—C(35)—N(31)	124 (5)

Roman numerals as superscripts refer to the following equivalent positions relative to the atoms at x, y, z :

(i) $\frac{1}{2} - x, \frac{1}{2} + y, 1 - z$; (ii) $\frac{1}{2} - x, y - \frac{1}{2}, 1 - z$.

The tpt functions as both a tridentate and monodentate ligand to Co(1) and Co(2) respectively. One triazine and two pyridyl N atoms of the ligand coordinate to Co(1) [mean Co—N 2.07 (3) Å] and a distorted octahedron is completed by Cl(11) and Cl(12) (Co—Cl 2.23 and 2.55 Å) and a water molecule [Co—O(1) 2.19 Å]. Co(2) is surrounded by three Cl atoms [mean Co—Cl 2.22 (1) Å] and the remaining pyridyl N atom of the ligand [Co—N(31) 1.99 Å] forming a distorted tetrahedron. Cl(12) bridges Co(1) and Co(2) of adjacent molecules [Co(1)—Cl(12)—Co(2) 124.1 (4)°] to form molecular chains parallel to [010]. It is of interest that such a bridge exists in the presence of the uncoordinated water molecule O(2).

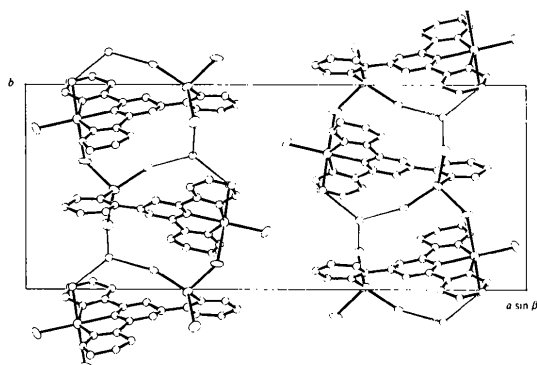


Fig. 2. Molecular packing in the crystal.

We had suggested (Vagg, Warrener & Watton, 1969) that in this type of compound the ligand may be acting as both tridentate and bidentate to the two metal atoms. Durham, Frost & Hart (1969) have argued that coordination of tpt to more than one metal atom would not be expected on electronic and steric grounds. The ligand functions as an approximately planar tridentate to Co(1) (Table 3, plane 1). Distortions caused by this coordination are similar to those described in the Ni complex (Barclay, Vagg & Watton, 1977*a*). The third pyridyl ring is rotated 38° around the bond to the triazine centre. Steric interaction of H(12) with Co(2) would not allow the ligand to act as a planar bidentate to that metal; however, the close N(3)—Co(2) distance of 2.75 (4) Å indicates a weak interaction between these atoms. This is evidenced also by the angular distortions in the coordination sphere of Co(2) towards a trigonal bipyramid (Table 2 and Fig. 3).

Other distortions in the ligand are apparent. The molecule is bent along the N(1)—C(34) direction (Fig. 2) such that the C(31)—C(34) direction intersects at 15° the tridentate plane (Table 3, plane 1). This effect is particularly evident in the non-planarity of the central *s*-triazine ring (Table 3, plane 2). The ring adopts a distinct chair conformation; the planes defined by N(1), C(1) and C(2), and N(2), N(3) and C(3) intersect that defined by C(1), C(2), N(2) and N(3) (Table 3, planes 3, 4 and 5) at 5 and 17° respectively. The three pyridyl rings show no significant deviation from planarity (Table 3, planes 6, 7 and 8).

Table 3. *Least-squares planes and their equations given by $lX' + mY' + nZ' - p = 0$, where X' , Y' and Z' are orthogonal coordinates related to the atomic coordinates X , Y and Z by $X' = X \sin \beta$, $Y' = Y$ and $Z' = Z + \cos \beta$*

Deviations (Å) of atoms from the planes are given in square brackets. Values in parentheses are standard deviations calculated solely from errors in atomic coordinates.

	<i>l</i>	<i>m</i>	<i>n</i>	<i>p</i>
Plane 1: Co(1), N(1)—(3), C(1)—(3), N(11), N(21), C(11)—(15), C(21)—(25) [Co(1) 0.12; N(1) 0.02; N(2), N(11) 0.06; N(3), C(13) 0.13; N(21), C(21) 0.05; C(1) 0.07; C(2) 0.09; C(3) 0.11; C(11), C(12) 0.04; C(14) 0.04; C(15) 0.08; C(22) 0.02; C(23) 0.05; C(24) 0.09; C(25) 0.11; C(31) 0.17; C(34) 0.64]	0.1102	0.9069	-0.4067	4.6218
Plane 2: C(1)—(3), N(1)—(3) [N(1) 0.001 (35); N(2) 0.049 (35); N(3) 0.067 (30); C(1) 0.024 (43); C(2) 0.011 (45); C(3) 0.080 (41); Co(1) 0.186 (7)]	0.1001	0.9368	-0.3351	4.6729
Plane 3: N(1), C(1), C(2)	0.0708	0.9388	-0.3370	4.4306
Plane 4: N(2), N(3), C(3)	-0.1309	0.9467	-0.2942	3.2367
Plane 5: N(2), N(3), C(1), C(2) [C(1) 0.008 (43); C(2) 0.008 (45); N(2) 0.008 (35); N(3) 0.008 (30); N(1) 0.052 (35); C(3) 0.172 (41)]	0.1585	0.9271	-0.3397	5.0773
Plane 6: N(11), C(11)—(15) [N(11) 0.005 (29); C(11) 0.027 (46); C(12) 0.054 (42); C(13) 0.054 (45); C(14) 0.022 (41); C(15) 0.010 (42); Co(1) 0.037 (7)]	0.1708	0.9086	-0.3811	5.0978
Plane 7: N(21), C(21)—(25) [N(21) 0.038 (30); C(21) 0.014 (42); C(22) 0.010 (40); C(23) 0.011 (44); C(24) 0.015 (46); C(25) 0.040 (42); Co(1) 0.049 (7)]	0.0536	0.8953	-0.4421	3.9178
Plane 8: N(31), C(31)—(35) [N(31) 0.028 (29); C(31) 0.009 (36); C(32) 0.034 (38); C(33) 0.024 (44); C(34) 0.012 (43); C(35) 0.040 (45); Co(2) 0.126 (7)]	-0.0036	0.9507	0.3101	4.3796
Plane 9: N(1), N(2), C(1), C(2) [N(1) 0.019 (35); N(2) 0.009 (35); C(1) 0.009 (43); C(2) 0.018 (45); N(3) 0.049 (30); C(3) 0.123 (41)]	0.1241	0.9298	-0.3466	4.8296
Plane 10: O(2), N(1), C(2)	0.9452	0.0556	0.3216	8.2564

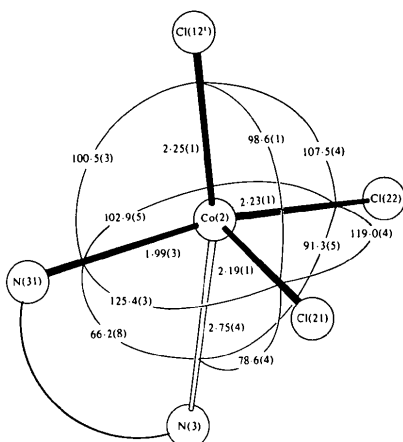


Fig. 3. The coordination sphere of Co(2).

Table 4. Close intermolecular contacts (Å) to the water molecule O(2)

Van der Waals contact distances (*Handbook of Chemistry and Physics*, 1974) are given in parentheses. Numbered interactions are shown in Fig. 1.

Interaction	Atom at		
1	N(1)	(x, y, z)	2.97 (3.25)
2	C(2)	(x, y, z)	3.11 (3.25)
3	N(3)	($\frac{1}{2} - x, \frac{1}{2} + y, 1 - z$)	3.17 (3.25)
4	O(1)	(x, y, z)	2.59 (2.80)
5	Cl(22)	($\frac{1}{2} - x, \frac{1}{2} + y, 1 - z$)	3.09 (3.20)
6	Cl(21)	(x, y, z)	3.06 (3.20)

The uncoordinated water molecule O(2) has close intermolecular contacts with O(1), Cl(21), Cl(22ⁱ), N(1), C(2) and N(3ⁱ) (Fig. 1 and Table 4). Of particular interest is the close contact [2.95 (4) Å] of O(2) with the N(1)–C(2) bond of the triazine ring. The water molecule sits directly above this bond (Table 3, planes 9 and 10 intersect at 87°), and is some 0.3 Å nearer than the van der Waals contact distance (*Handbook of Chemistry and Physics*, 1974).

It has been demonstrated that molecular water will add to the C–N bond of coordinated *N* heterocycles to form covalent hydrate species (Gillard & Williams,

1977). We have reported (Johnston, Vagg & Watton, 1978) that in some Co^{II} complexes of *s*-triazine there is evidence for a strong interaction between water and the coordinated base. The high sensitivity of *s*-triazine towards attack by water (Grundmann & Kreutzberger, 1954), the observed hydrolytic cleavage of part of the central triazine residue of metal complexes of tpt (Lerner & Lippard, 1976), and the formation of a covalent hydrate of *s*-triazine in acid solutions (Korolev, Mal'tseva & Andronova, 1975) are known. The structure of the unstable compound described here suggests that hydrolytic attack occurs at one of the central coordinated C–N bonds of the *s*-triazine residue in this complexed form.

References

- BARCLAY, G. A., VAGG, R. S. & WATTON, E. C. (1977a). *Acta Cryst.* B33, 3487–3491.
- BARCLAY, G. A., VAGG, R. S. & WATTON, E. C. (1977b). *Acta Cryst.* B33, 3777–3781.
- BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS*. Report ORNL-TM-305. Oak Ridge National Laboratory, Tennessee.
- COPPENS, P., LEISEROWITZ, L. & RABINOVICH, D. (1965). *Acta Cryst.* 18, 1035–1038.
- DURHAM, D. A., FROST, G. H. & HART, F. A. (1969). *J. Inorg. Nucl. Chem.* 31, 571–574.
- GILLARD, R. D. & WILLIAMS, P. A. (1977). *Transition Met. Chem.* 2, 14–18.
- GRUNDMANN, C. & KREUTZBERGER, A. (1954). *J. Am. Chem. Soc.* 76, 5646–5650.
- Handbook of Chemistry and Physics* (1974). 55th ed., p. D-157. Cleveland, Ohio: Chemical Rubber Company.
- International Tables for X-ray Crystallography* (1962). Vol. III, pp. 202–205. Birmingham: Kynoch Press.
- JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794, revised 1971. Oak Ridge National Laboratory, Tennessee.
- JOHNSTON, R. D., VAGG, R. S. & WATTON, E. C. (1978). *Inorg. Chim. Acta*, 26, 103–106.
- KOROLEV, B. A., MAL'TSEVA, M. A. & ANDRONOVA, N. A. (1975). *Zh. Obshch. Khim.* 45, 234–235.
- LERNER, E. I. & LIPPARD, S. J. (1976). *J. Am. Chem. Soc.* 98, 5397–5398.
- VAGG, R. S., WARRENER, R. N. & WATTON, E. C. (1967). *Aust. J. Chem.* 20, 1841–1857.
- VAGG, R. S., WARRENER, R. N. & WATTON, E. C. (1969). *Aust. J. Chem.* 22, 141–152.