Synthesis of the Complexes of S₃N₃Cl₃ with Cadmium(II) and Mercury(II)

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Complexes of trithiazyl trichloride, S₃N₃Cl₃, with Cd(CH₃COO)₂ and HgCl₂ were synthesized and analyzed. On the basis of its IR and X-ray powder spectra, it is revealed that both the complexes have tetragonal geometry. The antibacterial and toxic effect of these complexes on the albino rats was also tested.

Key Words: Synthesis, Trithiazyl trichloride, Complexes, Cadmium(II), Mercury(II).

INTRODUCTION

The complexes of trithiazyl trichloride (TTTCl), $S_3N_3Cl_3$ with Al(II), Mo(VI), Cu(II), Th(IV) and Zr(IV) have been reported¹⁻⁵. In continuation of our previous work⁶, X-ray diffraction studies of the complexes of $S_3N_3Cl_3$ with Cd(II) and Hg(II) are being presented.

RESULTS AND DISCUSSION

On the basis of alalytical analysis, m.w. determination and mass spectra, the complexes of TTTCl, synthesised with Cd(II) and Hg(II), have been formulated as $(S_3N_3Cl_3)_4$ Cd(CH₃COO)₂ and S_3N_3 Cl₃·HgCl₂ respectively. The IR spectra (Table-1) of the complexes possess two N—S \rightarrow Cd and two S—N \rightarrow Cd bands in $(S_3N_3Cl_3)_4$ ·Cd(CH₃COO)₂ and only two S—N \rightarrow Hg bands in S_3N_3 Cl₃·HgCl₂ inferring the quadridentated and bidentated linkage of S_3N_3 Cl₃ to Cd(CH₃COO)₂ and HgCl₂ respectively.

To elucidate the geometrical structure of the complexes, from their X-ray diffraction spectra (Table-2), recorded in 2θ range (10–70°), unit cell parameters, 'hkl' and 'd' were calculated. The values of 'd' observed resembles with the theoretical ones inferring its structure. The axial ratios, a_0 , b_0 and c_0 , were determined as:

$$\frac{a_0}{b_0} = \frac{\sin \phi_1}{\sin \phi_2}, \quad \frac{c_0}{a_0} = \frac{\sin \phi_3}{\sin \phi_4}$$

1894 Rani et al. Asian J. Chem.

TABLE-1
IR SPECTRAL DATA OF THE COMPLEXES

TTTCI·Cd	(CH ₃ COO) ₂	TTTCl.HgCl ₂		
Bands	Assignments	Bands	Assignments	
410 s	S—Cl	408	S—Cl	
449 b	N—S→M	5557	Hg—Cl	
513 s	S—CI	632	S—N→M	
557 wb	N—S→M	671	S—N→M	
615 b	S—N→M			
673 b	S—N→M			
715 s	S—N ring	736 s	S—N ring	
		1043 s	N—S—C1	
1109 s	N—S—Cl	1103 s	N—S—CI	
1155 s	N—S—CI	1157	N—S—Cl	
1314	N—S—CI	1300	N—S—CI	
1407 ws	N—S—Cl	1400	N—S—CI	
1571 b	CH ₃ COO ⁻			

The values $a_0 = b_0 = 7.5771$, $c_0 = 4.7254$ and $\alpha = \beta = 113.07^\circ$ and $\gamma = 96.3^\circ$ are according to tetragonal geometrical array of both the complexes. Both the complexes are found to be active against all bacteria, except *E. coli*, when they were treated on the *S. albus, S. aureus* (gram +ve), *B. pulminas* and *E. coli* (gram -ve) bacteria. Toxicity of the complexes was tested on albino rats by using 0.1 mL of test solution (5 mg/mL)/kg wt. and the complexes are found to be toxic in nature (Table-3).

EXPERIMENTAL

AnalaR grade chemicals were used throughout the present work. TTTCl was synthesized³ by chlorination of S_4N_4 ⁸ dissolved in CS_2 kept at 0°C. The resulting blue solid, $S_3N_3Cl_3$ (500 mg) was mixed with 500 mg of $Cd(CH_3COO)_2$ and $HgCl_2$ in DMF separately and refluxed for 24 h. The resultant solids were separated, washed successively with DMF, ethanol and ether, dried and stored in vacuum desiccator over fused $CaCl_2$.

TABLE-2 XRD PATTERN OF THE COMPLEXES

S.No.	TTTCl·Cd(CH ₃ COO) ₂			TTTCl·HgCl ₂		
	2θ (°)	hkl	d(Å) obs. (cal.)	2θ (°)	hkl	d(Å) obs.(cal)
1.	12.0	100	7.3749 (7.3688)	10.6	100	8.3431 (8.3387)
2.	15.4	110	5.7572 (5.7487)	15.3	110	5.7919 (5.7861)
3.	20.5	111	4.3328 (4.3286)	17.0	111	5.2158 (5.2111)
4.	25.4	200	3.5070 (3.5038)	20.5	200	4.3328 (4.3286)
5.	27.0	210	3.3027 (3.2995)	25.5	210	3.4935 (3.4992)
6.	29.9	211	2.9887 (2.9857)	26.3	211	3.3515 (3.3857)
7.	33.9	220	2.6446 (2.6420)	29.7	220	3.0083 (3.0054)
8.	36.4	300	2.3444 (2.4461)	31.2	300	2.8670 (2.8642)
9.	39.1	310	2.3040 (2.3018)	35.6	311	2.5221 (2.5197)
10.	41.3	311	2.1863 (2.1842)	38.8	320	2.3212 (2.3189)
11.	44.0	320	2.0582 (2.0562)	43.7	400	2.0716 (2.0690)
12.	48.8	400	1.8664 (1.8645)	51.4	421	1.7779 (1.7767)
13.	52.4	411	1.7463 (1.7446)	54.4	422	1.6867 (1.6852)

TABLE-3 TOXIC AND ANTIBACTERIAL TEST OF THE COMPLEXES

	gram +ve Bacteria		gram -ve Bacteria		Toxicity	
Complexes	S. Albus	S. Aureus	B. pulminas	E. coli	doses	Inference
TTTCl·Cd(CH ₃ COO) ₂	+2.16	+1.74	+2.72		0.1 mL	Expired after 1 min
	+2.10	+1.70	+2.70		0.2 mL	Expired after 30 s
TTTCl·HgCl ₂	+2.60	+2.60	+1.85		0.1 mL	Expired at once
	+2.65	+2.65	+1.80		0.2 mL	Expired at once

1896 Rani et al. Asian J. Chem.

The IR and X-ray diffraction spectra of the complexes were recorded subsequently on 820/P.C. (KBr) and ISO Deveflux 2002 X-ray powder diffractometer, using Cu filment as source of radiation ($\lambda = 1.5418 \text{ Å}$).

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