



**Figure 4.** Burrow openings on the surface in sandstone from Jhuran Formation, Jurassic of Kutch. Note the similarity with burrow openings produced by *Umbonium*.

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## SPECTRAL STUDY OF THE C - X SYSTEM OF TRANSIENT MERCURY BROMIDE

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THE study of mercury-halides has gained considerable attention due to its importance in high power electronic lasers in visible and UV regions. In these

molecules, ground state has weak binding, and therefore there is maximum possibility of population-inversion.

Spectroscopic studies of mercury halides are still incomplete. Vibrational analysis of the C-X system of transient HgBr, lying in the region 2940-2730 Å, has been studied due to the very complex nature of its emission spectrum. The first extensive study of this system was by Wieland<sup>1-5</sup>, who ascribed these bands to triatomic species HgBr<sub>2</sub> on account of the complex structure of bands. Later this system was analysed<sup>6-9</sup> and explained as due to diatomic species. These analyses were unconvincing according to Huber and Herzberg<sup>10</sup>.

Recently Rai *et al*<sup>9</sup> investigated the C-X system at high resolution on 35' concave grating spectrograph and the bands were assigned due to a diatomic emitter although a large number of bands remained unassigned. Hence their vibrational assignments appeared doubtful due to the following reasons:— (i) The band heads were not sharp as are expected to appear in the spectrum of diatomic molecule; (ii) All the sub-bands associated with each main band remained unassigned even at a lower resolution (on 21' concave grating spectrograph in second order at reciprocal dispersion 1.23 Å/mm). No reason has been given for these multiple band-heads. (iii) Only 60 bands have been reported and analysed in the C-X system. Band-head positions of (2, 0) and (2, 1) bands have been reported at wave numbers 35210.51 cm<sup>-1</sup> and 35126.61 cm<sup>-1</sup> respectively (difference: 83.91 cm<sup>-1</sup>). This horizontal interval is inconsistent with other studies. The same inconsistency exists in vertical intervals. Thus the values of Rai *et al* does not show proper fitting of the bands. Many other discrepancies appear in the analysis. So the prediction by Wieland for ascribing the C-X system to the triatomic emitter may be true and this is confirmed in the present investigation.

The emission spectrum was recorded by exciting a pure sample of mercuric bromide (BDH) with a 1/2 kW, 30-40 MHz high frequency oscillator in an electrodeless discharge/using a 100 W microwave generator (2450 MHz). When the discharge appeared intense sky-blue, all the bands could be excited and were well developed. The spectrum was recorded on medium quartz, Littrow, 21' concave grating and 35' concave grating spectrographs separately on Q<sub>1</sub> and Q<sub>2</sub> Ilford plates of 2" × 10" size. Iron arc spectrum run at low current in air was superimposed as standard for the measurements of the plates. The measurements were carried out with a Carl-Zeiss (Abbe) comparator. Several spectro-

**Table 1** Intense band-heads of C-X system of transient HgBr with previous assignment as diatomic emitter, observed band head positions, calculated band head positions as triatomic emitter, visual intensity (I), calculated head separations and isotopic shift (as diatomic) and present assignment as triatomic emitter (on 2I' concave-grating in II order)

Previous assignment of the bands as diatomic ( $\nu', \nu''$ )	Band-Head positions				Calculated isotopic-shift Hg <sup>81</sup> Br-Hg <sup>79</sup> Br (cm <sup>-1</sup> )	Present assignment as triatomic emitter ( $\nu_1' \nu_2' \nu_3' - \nu_1'' \nu_2'' \nu_3''$ )
	Observed experimentally $\nu$ (cm <sup>-1</sup> )	Calculated as triatomic emitter $\nu$ (cm <sup>-1</sup> )	I	Calculated $P_{\text{head}} - Q_{\text{head}}$ (cm <sup>-1</sup> )		
(0,2)	343	97.1	343	97.6	4	(110-310)
	344	00.6	344	00.6	4	(022-004)
		04.5		01.6	3	(320-242)
		08.6		09.6	3	(012-212)
		15.0		14.7	2	(000-200)
(1,3)	344	86.2	344	84.7	4	(110-230)
		89.7		86.7	4	(011-131)
		94.9		96.7	4	(012-132)
	345	03.8	345	01.7	4	(000-320)
(0,1)	345	83.1	345	86.7	6	(012-112)
		90.3		91.6	5	(000-100)
	346	00.1	346	00.0	5	(100-200)
(1,2)		10.6		11.6	5	(002-102)
	346	68.9	346	68.7	6	(040-040)
		74.2		73.7	6	(012-032)
		77.9		78.7	5	(000-020)
(0,0)		87.1		86.7	4	(100-120)
	347	68.8	347	68.7	10	(000-000)
		74.9		76.6	9	(100-100)
		83.9		84.0	9	(200-200)
(1,1)		92.9		92.6	9	(300-300)
	348	58.1	348	58.7	4	(041-001)
		68.4		68.7	4	(042-002)
		78.5		78.7	3	(043-003)
(2,2)		86.9		88.0	3	(044-004)
	349	37.8	349	35.7	2	(320-002)
		40.9		38.7	3	(111-011)
		48.4		48.7	3	(112-012)
(1,0)		53.8		53.7	3	(100-000)
	350	36.9	350	36.7	8	(002-040)
		40.8		39.7	8	(002-100)
		44.7		43.7	8	(141-001)
(2,1)		68.1		64.7	4	(104-142)
	351	21.2	351	21.7	5	(014-032)
		33.4		33.7	4	(212-012)
		42.5		38.7	4	(200-000)
	48.5		48.7	4	(201-001)	

grams with different exposures and different slit-widths were recorded and each was measured many times. The band-head positions are expected to be

accurately determined to within  $\pm 0.1 \text{ cm}^{-1}$  for sharp bands and  $\pm 0.5 \text{ cm}^{-1}$  for broad bands.

In general, the bands are violet-degraded at low



dispersions. The bands from 2918 Å to 2838 Å appear sharp, single-headed and exhibit certain features which may be due to isotopic effect. From 2838 to 2813 Å, they do not possess sharp bands and below 2813 Å, they are in pairs with constant separation. All the attempts to assign these bands as diatomic emitter failed.

Intense band-heads of C-X system of transient HgBr are observed on 21' concave grating spectrograph in II order (table 1). The calculated ( $P_{\text{head}} - Q_{\text{head}}$ ) separation and isotopic-shifts (Hg<sup>81</sup>Br-Hg<sup>79</sup>Br) were obtained to account for these observed sub-band-heads separations for ascribing the bands to diatomic emitter. It is evident from the table that the observed band-head separations do not match with the above two calculations. This leads us to conclude that these bands are not due to diatomic HgBr. The emitter of these bands is definitely triatomic HgBr<sub>2</sub> as all the sub-band-heads, appearing with each main strong band, have been successfully explained with the present assignments in table 1, which gives the symmetric, bending and antisymmetric stretch frequencies for the upper and lower states of triatomic HgBr<sub>2</sub> emitter. The vibronic splitting of (012-212), (110-230), (100-120), (111-011) and (112-012) bands on 35' grating confirms the present assignment of the bands as triatomic emitter.

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### COORDINATION POLYMERS OF COBALT(II), NICKEL(II), COPPER(II), ZINC(II) AND CADMIUM(II) WITH 3-ALLYL-1-(2-MERCAPTO-4-OXO-3(4H)-QUINAZOLINYL)-2-THIOPSEUDOUREA

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COBALT(II), nickel(II), copper(II), zinc(II) and cadmium(II) complexes with 3-allyl-1-(2-mercapto-4-oxo-3(4H)-quinazolinyl)-2-thiopseudourea (H<sub>2</sub>L) have been synthesized and characterized on the basis of analytical, thermal, conductance, magnetic and spectral (IR, NMR, ESR and electronic) data. The data indicate the formation of ligand bridged polymeric octahedral complexes in which the ligand behaves as a pentadentate biprotic ligand. The sixth coordination position has been occupied by the water molecule.

The complex formation with 2-mercaptoquinazolin-4(3H)-one (figure 1) takes place through the nitrogen atom at position 1 and sulphur atom of the mercaptan group<sup>1</sup>. There are reports of oxygen also taking part in coordination<sup>2</sup>. Extensive work has been done in the field of metal complexes with its 3-substituted alkyl/aryl derivatives. The studies with potentially donor group at position 3 have not received much attention. The present communication reports the coordination polymers of cobalt(II), nickel(II), copper(II), zinc(II) and cadmium(II) with 3-allyl-1-(2-mercapto-4-oxo-3(4H)-quinazolinyl)-2-thiopseudourea (H<sub>2</sub>L).

3-Allyl-1-(2-mercapto-4-oxo-3(4H)-quinazolinyl)-2-thiopseudourea (H<sub>2</sub>L) was prepared by heating a mixture of allylthiocyanate (0.60 g) and 3-amino-2-mercaptoquinazolin-4(3H)-one<sup>3</sup> (1 g) on a steam bath for 2 hr. The solid mass was triturated with ethanol (2 ml) and collected under suction. It was crystallized from ethanol. M. P. 210°C. Characterization data: Found S = 21.81, N = 19.26; calculated for C<sub>12</sub>H<sub>12</sub>N<sub>4</sub>OS<sub>2</sub> S = 21.92, N = 19.18.

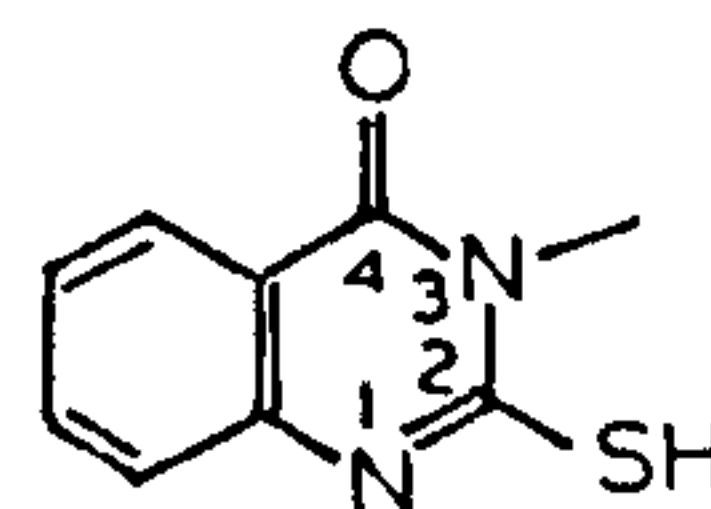


Figure 1.

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