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The Structure of Mercuric Amidobromide

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The structure of $HgNH_2Br$, similar to that of $HgNH_2Cl$, consists of infinite chains of alternating Hg and NH_2^+ with linear bonds about Hg and tetrahedral bonds about N. The unit cell is orthorhombic, C_{2v}^1–$P2mm$, with $a = 5{\cdot}439$, $b = 4{\cdot}487$ and $c = 6{\cdot}761$ Å. The Hg–N bond distance is 2·07 Å. The N–H · · · Br distance is 3·36 Å, based on the assumption that the Br · · · Br distance is 3·90 Å.

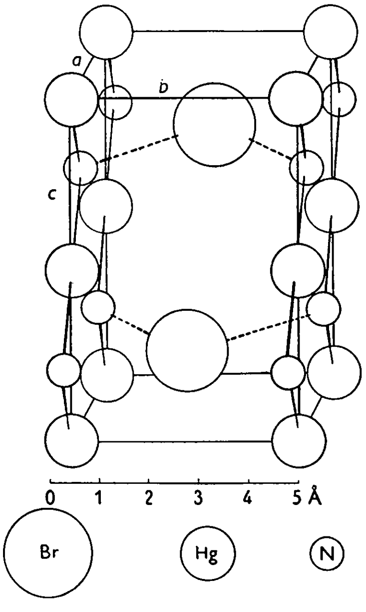

Fig. 1. The structure of $HgNH_2Br$.

Because the structure of orthorhombic $HgNH_2Cl$ was determined from powder photographs only (Lipscomb, 1951*b*), and because of the relatively small scattering of N and Cl as compared with Hg, we felt that an investigation of $HgNH_2Br$ should be made. The results of this investigation, which is part of more general chemical studies of the reactions of Hg(*I*) compounds with ammonia, show that $HgNH_2Br$ has the same structure as that proposed for $HgNH_2Cl$. In addition, values have been determined for the Hg–N bond distance, and for the N–H · · · Br hydrogen-bond distance.

A sample of $HgNH_2Br$ was prepared by the reaction of 150 ml. of 14N aqueous ammonia with 2 g. of Hg_2Br_2. The diffraction pattern from this powdered sample was taken by means of a General Electric XRD-3 unit with the use of a Geiger counter for recording the diffracted Cu $K\alpha$ radiation. Integrated intensities were measured from the tracing by the usual method.

The diffraction pattern was satisfactorily indexed on an orthorhombic unit cell with

$$a = 5{\cdot}439,\ b = 4{\cdot}487 \ \text{ and } \ c = 6{\cdot}761\ \text{Å},$$

all $\pm 0{\cdot}005$ Å ($\lambda = 1{\cdot}5418$ Å). Comparison of these unit-cell dimensions with those of $HgNH_2Cl$ confirms the proposed atomic arrangement (Fig. 1) in a striking way. The values for $HgNH_2Br$ are greater by 0·27 Å for *a*, 0·13 Å for *b*, and 0·07 Å for *c* than those for $HgNH_2Cl$. It should be noted that binding in the *a* direction is weakest, being chiefly dispersion forces, binding in the *b* direction is by hydrogen bonding, while binding in the *c* direction occurs through the relatively strong covalent bonds.

Comparison of the observed and calculated spacings and intensities is shown in Table 1. Calculated intensities include the contributions of all atoms. The usual Lorentz, polarization and multiplicity factors have been included. Atomic positions and parameters are:

2 Hg at $0, 0, 0;\ 0, 0, \frac{1}{2}$.
2 N at $0{\cdot}22, 0, \frac{1}{4};\ 0{\cdot}78, 0, \frac{3}{4}$.
2 Br at $0{\cdot}32, \frac{1}{2}, \frac{3}{4};\ 0{\cdot}68, \frac{1}{2}, \frac{1}{4}$.

These parameters were determined from the assumptions of tetrahedral bond angles about N, and a Br · · · Br distance of 3·90 Å (Pauling, 1942, p. 189). The space group is thus C_{2v}^1–$P2mm$. This structure corresponds with that proposed for $HgNH_2Cl$, whereas the alternative structure described as a possibility for $HgNH_2Cl$ can be conclusively eliminated for $HgNH_2Br$ by comparison of the observed intensities for (101) and (011) with the calculated values. For this alternative structure the calculated intensities are zero for (101) and 21 for (011), in complete disagreement with the observations.

Because single crystals were not available, the parameter values for N and Br cannot be considered as particularly accurate. However, two interatomic distances of interest may be determined from the cell dimensions. Based on the assumption of tetrahedral angles about N, the Hg–N bond distance is 2·07 Å. This value may be compared with the values of 2·07 Å and 2·05 Å found in $Hg_2NOH.2H_2O$ (Lipscomb, 1951*a*) and $HgNH_2Cl$ (Lipscomb, 1951*b*). Based on the assumption of a van der Waals contact of 3·90 Å between Br atoms, the N–H · · · Br distance is 3·36 Å, which is 0·1 Å shorter than the sum of the van der Waals radii (Pauling, 1942, p. 189) and therefore supports the assumption of a hydrogen bond in this direction.

Table 1. *Crystal data for* $HgNH_2Br$

hkl	d_c	I_c	d_o	I_o
001	6·655	0	—	< 3
100	5·353	71	5·367	49
010	4·392	16	4·421	18
101	4·171	12	4·173	15
011	3·681	0	—	< 3
110	3·407	104	3·411	52
002	3·328	8	3·331	8
111	3·033	22	3·034	21
102	2·826	58	2·829	40
200	2·676	73	2·661	50
012	2·658			
201	2·483	3	—	< 3
112	2·381	36	2·381	33
210	2·289	35	2·289	38
003	2·219	0	—	< 3
020	2·209	23	2·212	20
211	2·164	3	—	< 3
021	2·096	3	—	< 3
202	2·085	31	2·086	38
103	2·049	2	—	< 3
120	2·042	12	2·041	17
013	1·982	0	1·979	< 3
121	1·952	3	1·951	4
212	1·886	17	1·885	12
113	1·859	2	1·859	7
022	1·840	4	1·840	4
300	1·784	10	1·782	10
122	1·740	24	1·740	20
311	1·723	0	—	< 2
203	1·708	1	—	< 2
220	1·703	5	1·702	3
004	1·664	10	1·665	10
310	1·654	3	1·652	7
221	1·650	2	—	< 2
311	1·605	0	—	< 2
213	1·593	1	1·605	2
104	1·589	5	1·591	8
302	1·572	3	1·571	6
023	1·565	0	—	< 2
014	1·557	3	—	< 2
222	1·516	23	1·516	21
123	1·502	1	—	< 2

Table 1 (*cont.*)

hkl	d_c	I_c	d_o	I_o
114	1·495	17	1·496	17
312	1·481	24	1·480	18
030	1·472	1	—	< 2
031	1·438	0	—	< 2
130	1·420	7	1·419	6
204	1·413	2	—	< 2
303	1·390	0	—	< 2
131	1·389	1	—	< 2
320	1·388	8	1·387	7
321	1·359	0	—	< 2
223	1·351	1	—	< 2
032	1·346	21	1·346	24
214	1·346			
400	1·338	2	—	< 2
005	1·331	0	—	< 2
024	1·329	8	1·330	15
313	1·326	0	—	< 2
401	1·312	1	—	< 2
132	1·306	5	1·306	5
105	1·303	0	—	< 2
230	1·290	11	1·290	12
124	1·290			
322	1·281	8	1·281	8
410	1·281			
015	1·275	0	—	< 2
231	1·266	0	—	< 2
411	1·258	1	—	< 2
402	1·242	4	—	< 2
115	1·240	1	—	< 2
033	1·227	0	—	< 2
304	1·217	6	1·217	4
232	1·203	14	1·194	12
133	1·196			
412	1·195			
205	1·192			
224	1·190			
323	1·177	3	1·174	6
314	1·173			
215	1·150	3	1·144	4
403	1·146			
420	1·144			

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