

Rigid Covalent Atomic Groups in Precrystallization Phase for Hg-containing Compounds

Victor V. Atuchin, Stanislav V. Borisov, Svetlana A. Magarill, and Natalia V. Pervukhina

Abstract—During crystal chemical analysis of about fifty mercury-containing compounds the atomic groups same from structure to structure were found. Such atomic groups, namely $[\text{Hg}_4\text{O}]$ oxo-centered tetrahedron and r -octahedron $[\text{Hg}_6\text{O}_2]$, are covalently bonded. Quantum-chemical calculations prove stability of these ‘rigid’ atomic groups that are assumed to be formed in the beginning of crystallization. Thus, mechanism of crystallization proposed includes mutual arrangement of isolated or joint-like linked rigid atomic groups and finally their regular packing. At that point symmetry of these rigid atomic groups becomes subgroup of space group of the whole structure.

Index Terms—Crystal structure, mercury, minerals, coordination.

I. INTRODUCTION

Mercury compounds are key materials for many applications in micro- and nanoelectronics, photonics and nonlinear optics [1-7]. Because of chemical activity and oxidation state variability of mercury ions in nature many complex mercury-containing minerals are found in the earth-crust [8-12]. Understanding of crystal chemistry of mercury-bearing minerals and release ways for the hazardous components are of great importance for the environment keeping. Several new mercury-containing crystals have been discovered over recent years in the oxide and halcogenide systems that greatly extends the spectrum of effective materials for different applications [13-21].

Generally, mercury oxides, oxo- and chalcogenides are known to have intriguing, complex and multifarious structural and crystal chemistry. Mercury atoms can be bonded to oxygen, chalcogen, halogen or some other atoms both in covalent or ionic manner, be bonded to metal atoms to form mono- ($[\text{Hg}_2]^{2+}$ dumbbells, $[\text{Hg}_3]^{4+}$ triangles etc.) and hetero-nuclear clusters with silver, lead and several other metal atoms [22,23]. The crystal chemistry of mercury-containing compounds is of additional interest owing to ecological reasons concerning the occurrence of these compounds in the earth’s crust, water and atmosphere.

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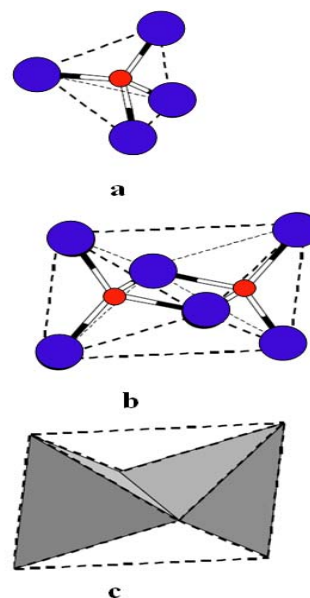


Fig. 1. Undistorted (a) $[\text{Hg}_4\text{O}]$ cationic tetrahedron and (b) $[\text{Hg}_6\text{O}_2]$ r -octahedron, i.e. a pair of $[\text{Hg}_4\text{O}]$ cationic tetrahedra, sharing an edge (c). Dashed lines show convex shape of the atomic groups.

Some features of crystal chemistry for compounds containing divalent mercury, oxygen, chalcogen and halogen atoms were investigated earlier and structural principles of formation for these compounds were proposed. It was shown that linear Y–Hg–Y groups, where Y are O, N, S, Se or Te atoms, are typical building blocks in crystal structures of most compounds. The groups are usually characterized by a YHgY bond angle of about 180° and shortened contact Hg–Y, e.g., Hg–O and Hg–S average distances are of 204 and 234 pm, respectively. Present study is aimed to continue this analysis with accounting new mercury-containing crystals and reveal some specific structural features general for this chemical class.

II. HG-CONTAINING COMPOUNDS

During crystallochemical analysis of about fifty Hg-containing compounds so-called ‘rigid’ atomic groups were found by detailed observation of coordination of metal atoms by anions. These atomic groups are called ‘rigid’ owing to their interatomic distances and bond angles remaining practically unchanged over a number of structures. Chemical bonding in such groups is usually partly or totally covalent with comparatively short bond lengths. If in the crystal structure there are oxygen atoms, which do not comprise anions such as $[\text{PO}_4]^{3-}$, $[\text{SO}_4]^{2-}$, $[\text{SiO}_4]^{4-}$ etc., they usually form $[\text{Hg}_4\text{O}]$ cationic tetrahedra (Fig. 1) with Hg–Hg

and Hg-O

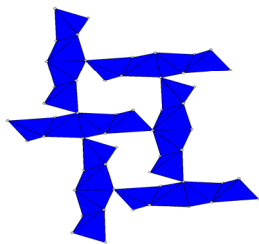


Fig. 2. Fragment of layer of doubled r-octahedra in β -Hg₆O₄Cl₄ crystal structure.

distances of 350 and 190-278 pm respectively [22-26]. In crystal structures of oxohalides such as Hg₆O₂Cl₂, α -Hg₃O₂Cl₂, Hg₂OI, Hg₇O₃Cl₂ etc., the 2 cationic tetrahedra share edges to form so-called 'r-octahedron' [Hg₆O₂] (Fig. 1b, c), or a pair of r-octahedra like in β -Hg₃O₂Cl₂ or Hg₆O₄Cl₄ [25] (Fig. 2). Centroids of r-octahedra usually coincide with symmetry centers. Thus, crystal structure may be described as

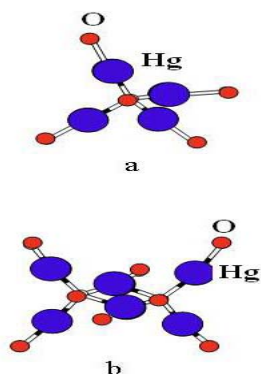


Fig. 3. Atomic groups (a) [Hg₄O₅]²⁻ and (b) [Hg₆O₈]⁴⁻ are chosen for quantum-chemical calculations.

regular close packing of such rigid atomic groups. The rest atoms occupy the voids of the packing. To prove that the [Hg₄O] cationic tetrahedra and [Hg₆O₂] r-octahedra are reasonable to be chosen as structure-forming groups the quantum-chemical calculations of model systems [Hg₄O₅]²⁻ and [Hg₆O₈]⁴⁻ were performed that are cationic tetrahedron and r-octahedron respectively with nearest covalent environment of mercury atoms (Fig. 3a,b). For calculations ZORA method [27] implemented in ADF program package [28] was used. The calculations show that [Hg₆O₈]⁴⁻ group is energetically more stable than single [Hg₄O₅]²⁻ group [29]. From geometrical point of view similar highly stable atomic groups containing metal-metal bonds were found in the various types of compounds. An 'unprecedented stability' of [Au₄OP₄] oxo-centered tetrahedron with covalent contacts of Au-Au = 335.9 pm, Au-O = 205.7 pm, Au-P = 222.5 pm etc. was reported for C₈₄H₈₄Au₄B₂F₈OP₄ crystal structure [30]. Stable [Au₄Rh₂O₂] r-octahedron, with interatomic distances Au-Au = 300.8 pm, Au-Rh = 298.4 and 302.0 pm, Au-O = 202.6 and 208.3 pm, Rh-O = 209.5 and 211.8 pm is found for [{(dien)Rh[μ -O(AuPPh₃)₂]₂][BF₄]] [31]. Let us consider crystal structure of AgHg₂PO₄ [32], which is an example of unusual combination of cationic and anionic groups. Cationic

[Hg₄Ag₂] r-octahedra consist of a pair of [Hg₂Ag₂] tetrahedra sharing Ag-Ag edge. Symmetry center is in the center of the Ag-Ag edge that coincides with the centroid of r-octahedron. In contrast to above-mentioned structures there is no oxygen atom in the center of the tetrahedron, and the tetrahedron is rather smaller (Hg-Hg = 260.8 pm; Ag-Ag = 282.4 pm; Hg-Ag = 284.0, 294.1 pm). Anionic fragment is a pair of [PO₄] tetrahedra related by symmetry center so that an empty octahedron of oxygen atoms separates them from each other (Fig. 4). Centroids of the complex anions and cluster cations are packed according to pseudo-BCC lattice.

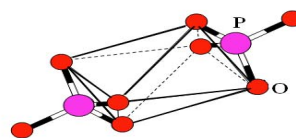


Fig. 4. An anionic part 2[PO₄] of AgHg₂PO₄ crystal structure. Two [PO₄]-groups that are trans to each other form an empty 'O₆ octahedron' (thin lines).

Recently tetragonal structure of tillmansite [Ag₃Hg][(V,As)O₄] was solved [33]. A mercury and three silver atoms statistically occupy vertices of each [Ag₃Hg] cationic tetrahedron, which is also empty. Cation-cation distances are 275.2 and 273.8 pm. The tetrahedral anions [(V,As)O₄] are interlaid with empty 'O₄ tetrahedra'. Both [(V,As)O₄] anions and O₄ tetrahedra share edges to form chain going along z-axis (Fig. 5). In the centers of both tetrahedra there are -4 special positions of *I*-4 space group. The rest two -4 special positions are in the centers of aforementioned empty cationic tetrahedron and also empty [Ag₃Hg] tetrahedron. The latter tetrahedron is elongated along z-axis. Its edges of about 3.5 Å tilted to ab-plane are an evidence of no strong chemical interactions between the metal atoms. Both tetrahedra share edges and are arranged in alternative order. Like in the AgHg₂PO₄ structure each pair of cationic tetrahedra may be considered as distorted 'empty' r-octahedron. In crystal structure the tapes of r-octahedra and tapes of anionic tetrahedra are interleaved in chess-like order as can be clearly seen in Fig. 5. Note that positions of the cations (Ag,Hg) and (V,As) form pseudo-FCC lattice. Sub-unit of the lattice is 2/5 times smaller than original tetragonal asymmetric unit.

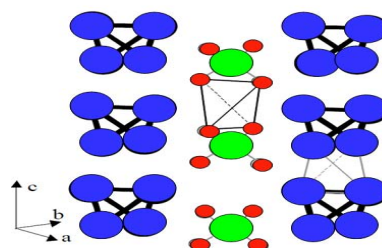


Fig. 5. Tillmansite (Ag₃Hg)(V,As)O₄ crystal structure. Chess-like packing of [Ag₃Hg] and [(V,As)O₄] tapes. Red, dark blue and green circles denote O, Ag and Hg, As and V atoms respectively.

We suppose that such rigid atomic groups, as r-octahedra are likely to exist even before crystallization if there are appropriate mercury and oxygen stoichiometric relationships, proper charge compensation components *etc.* This is

naturally because the forces that cause formation of rigid atomic groups are much stronger than the forces, responsible for crystallization or, other words, long-range order arrangement of atoms or centroids of the rigid atomic groups. Thus, the mechanism of the crystallization was proposed in Ref. [34], according to which mutual joint-like movement of nearest rigid atomic groups around the bonds between them yields to regular close packing (Fig. 2, 6). Centroids of the rigid atomic groups are fixed on crystallographic planes, which $dhkl$ are close to linear dimensions of the groups. We think that the arrangement of these groups gives main contribution to crystallization process just like in case of molecular compounds. Moreover, own point symmetry of rigid atomic groups should predetermine somehow the symmetry of a crystal structure, because these groups usually occupy highsymmetry special positions as one can see from the aforementioned examples.

III. CONCLUSION

Thus, the formation of mercury-containing crystal structures may be assumed to be the result of primarily the low-resolution (large d_{hkl}) ordering of the building blocks, the largest in size and mass, by a set of unique crystallographic planes or, in other words, by coordinate planes that form a translation-related sublattice of the building blocks [22,23,25,34]. At the same time, the coordinate planes of unique sublattices can arrange smaller building blocks and single atoms giving high-resolution ordering (smaller d_{hkl}). Some atoms of the large building blocks may also take part in the ordering of small building blocks. When the crystal structure has been formed, all sets of primarily unique sublattices of different combinations of atoms and rigid atomic groups have formed a general periodic lattice, which fits to all atoms and rigid atomic groups. The unit cell of the lattice includes an integer number of any subcell, while indices of all sets of planes are integers. Thus, all sets of planes become crystallographic.

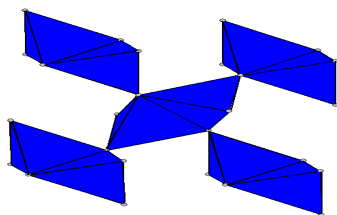


Fig. 6. Herringbone packing pattern of joint-like fitting r-octahedra along yz-plane in $-\text{Hg}_3\text{O}_2\text{Cl}_2$ crystal structure.

The stability of a crystal structure is known to depend on decreasing the degrees of freedom of the atoms in comparison with the initial chaotic arrangement. Another way to decrease degrees of freedom and, therefore, to minimize the energy of an atomic ensemble is in the symmetry relations between the ordering planes. This is the reason for atoms to occupy the special positions in a crystal structure and, thus, to stabilize it. The local point symmetry of a building block influences the space symmetry of a crystal structure as has been illustrated above.

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