

What Defines a Halide Perovskite?

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Over the last two decades, halide perovskites (HPs) have been identified as one of the most promising materials in photovoltaic and light-emitting devices.^{1,2} This has led to major breakthroughs in materials science^{3,4} but has also brought about a general misunderstanding and misuse of the term “perovskite”. In this Viewpoint, we will address the definition of a perovskite, with a main focus on the subgroup of perovskites that consist of heavier halides (Cl, Br, and I), both fully inorganic and hybrid organic–inorganic ones, as well as the many variants that can be found within this subgroup. In doing so, we will clarify what defines, in our opinion, a halide perovskite and discuss the commonly misnamed nonperovskite crystal structures.

A perovskite crystal lattice is defined as a network of corner-sharing BX_6 octahedra that crystallize with a general ABX_3 (or equivalent) stoichiometry, as is shown in Figures 1 and 2a.⁵

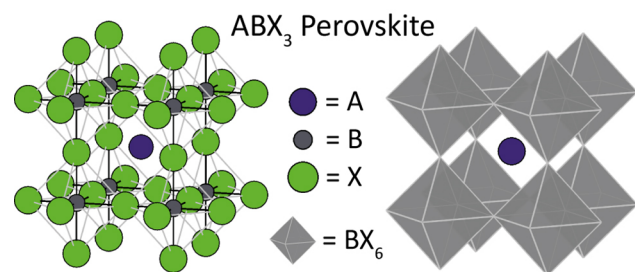


Figure 1. Standard depiction of the aristotype cubic perovskite. Shown in display styles evidencing either all the atoms (left) or only the BX_6 octahedral network and A atoms (right).

Deviations from this ABX_3 stoichiometry can be obtained when the A and B cation sites become partially or fully vacant (vacancy-ordered perovskites), or when they are replaced by a combination of other cations (with different valences but with an overall neutral charge balance), forming double or quadruple perovskites. The aristotype (the highest symmetric structure of a group of crystal structures)⁶ perovskite belongs to the $Pm\bar{3}m$ cubic space group, with $SrTiO_3$ (tausonite) usually considered the prime example. The vast majority of perovskites though have a reduced symmetry (hettotypes, i.e. structures that are similar to the aristotype, but with a lower symmetry)⁶ due to lattice distortions, distorted octahedra, ordered cations, vacancies, or the presence of organic cations or inorganic clusters.

The term “perovskite” was first coined by Gustav Rose in 1839 for the $CaTiO_3$ mineral, who named it after the Russian nobleman and mineralogist Count Lev Alekseyevich von

Perovski. Later, in 1926, it was first used as a general term for the crystal structure group by Victor Goldschmidt.³ In nature, perovskites are primarily found as oxides, with the majority being silicates (such as bridgmanite minerals),⁷ but they also exist as fluorides, chlorides, hydroxides, arsenides, and intermetallic compounds.⁵ While the number of natural perovskite minerals is limited, synthetic perovskites span across the whole periodic table in terms of elemental composition, and they can exist in many complex formulas such as metallic perovskites (e.g., $MgCNi_3$),⁸ hybrid organic–inorganic perovskites (e.g., $[CH_3NH_3]PbI_3$ and $[CH_3NH_3]Mn(HCOO)_3$),⁹ metal-free perovskites (e.g., $[DABCO][NH_4]I_3$ with MDABCO = *N*-methyl-*N'*-diazabicyclo[2.2.2]octonium),¹⁰ and even noble gas-based perovskites ($KSrXeNaO_6$).¹¹ This indicates that the perovskite is perhaps the most adaptable type of crystal lattice.

Inorganic Metal Halide Perovskites. The subgroup of perovskites (and ternary metal halides in general) that will be discussed in this Viewpoint have halides as their X anions. In the case of standard perovskites (that is, those with an ABX_3 stoichiometry) the B cations are divalent (like Pb^{2+} , or Sn^{2+}) and the A cations are large monovalent alkali metals (most commonly cesium) or small organic cations like methylammonium (MA) or formamidinium (FA). Because of the single charge of the anions in HPs, the A and B cations are limited to M(I) and M(II), respectively (not considering ordered or vacant perovskites).

While this Viewpoint will mainly concentrate on heavy metal-based halides, which generally have bandgaps in the visible spectrum and NIR (therefore they are of more interest for use in photovoltaic and light emitting devices), there is a vast group of first row transition metal fluoride perovskites, which can be interesting for lithium intercalation or as a host material for up- or down-conversion emission.^{12–14} One of these fluoride perovskites, $KMgF_3$ (parascandolaite),¹⁵ is also one of the few HPs that can be found in nature, and it crystallizes in a perfect cubic perovskite structure ($Pm\bar{3}m$). Therefore, $KMgF_3$ is a more suitable aristotype for HPs than $SrTiO_3$.⁵ Fluoride perovskites can also crystallize in a so-called “inverse perovskite” (which is not to be confused with antiperovskite), in which the A cation has a higher oxidation

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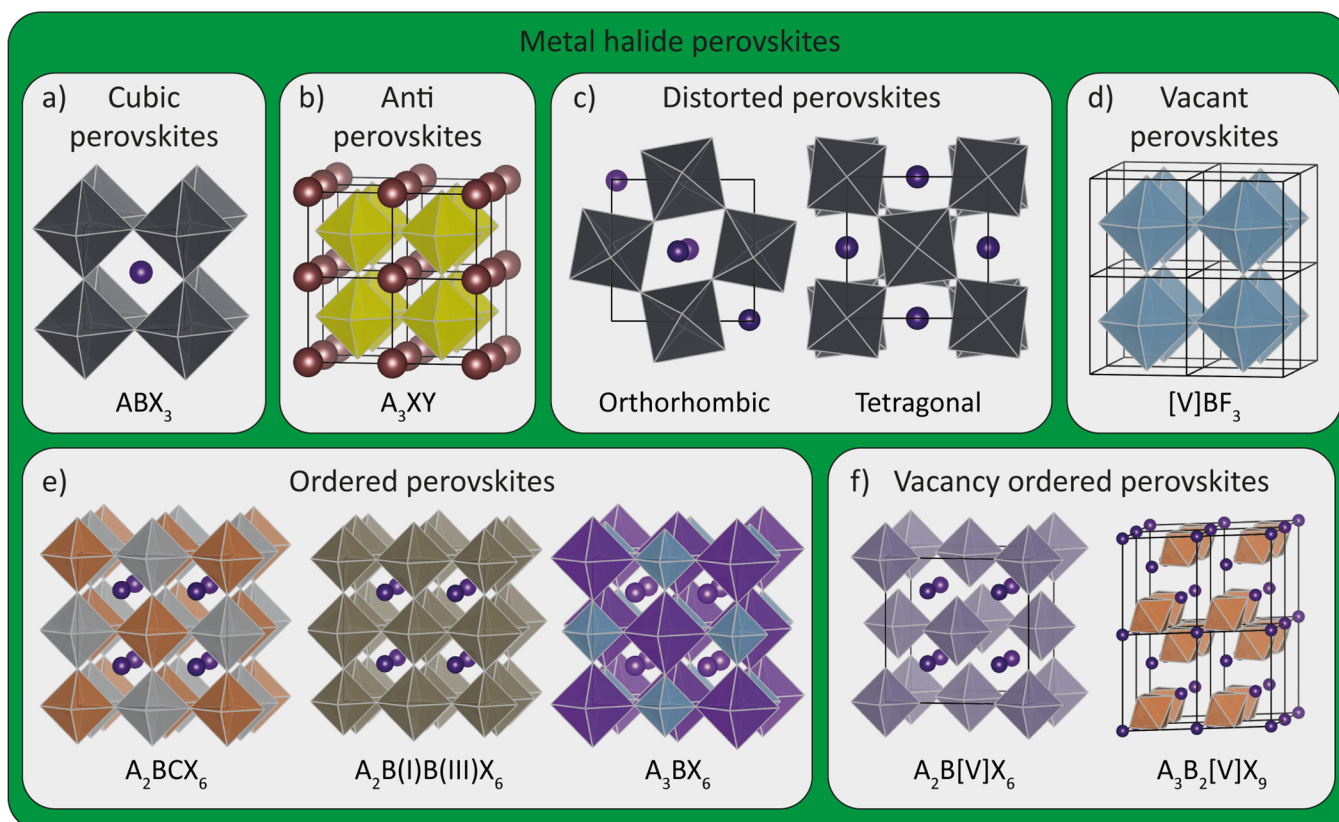


Figure 2. Overview of different halide perovskites. (a) Standard ABX_3 cubic halide perovskites. (b) Antiperovskites, with A being a monovalent metal (like Li^+ or Ag^+), X a halide, and Y a chalcogenide. (c) Common orthorhombic and tetragonal disordered perovskites, arising from the tilting of the octahedra. (d) Vacant BX_3 perovskites, like AlF_3 . (e) Ordered perovskites, where two M(II) metals are replaced by a M(I) and M(III) metal. (f) Vacancy-ordered perovskites, where a part of the B-site cations are replaced with a M(III) or M(IV) and vacancies.

state than the B cation, like in the case of $BaLiF_3$.¹⁶ This occurs only when the A cations (e.g., Ba^{2+} and Sr^{2+}) are very large and the B cations (e.g., Li^+) are very small. Moreover, these small B cations can only form perovskites with F^- and H^- ions. Finally, halide antiperovskites also exist, in which the A and B sites are occupied by anions (halide and chalcogenide respectively) and the X sites are occupied by a monovalent cation (as is shown in Figure 2b).^{17,18} Halide antiperovskites like Li_3OBr and Ag_3SI will not be discussed in this Viewpoint, as the halide is not part of the BX framework, but they certainly do classify as perovskites.

Fully inorganic, heavy metal HPs do not crystallize in the pure cubic perovskite crystal lattice. Rather, they exhibit a distorted lattice, resulting in hettotype structures. These distortions occur as a result of the size difference between the A, B, and X cations. Consequently, the individual octahedra tilt, which generally results in either orthorhombic (commonly referred to as the “ $GdFeO_3$ -type”)¹⁹ or tetragonal crystal structures (Figure 2c).¹⁹ Although these distortions are responsible for the lower crystal structure symmetry, the overall perovskite framework is preserved; therefore, these materials are classified as hettotypes of the perovskite group. In fact, even the original perovskite ($CaTiO_3$) exhibits a small distortion and does not actually crystallize in a “perfect” cubic perovskite structure.⁵

Several variants of the perovskite structure, and thus of ABX_3 stoichiometry, can be obtained by partially or fully replacing (ordering) or even removing A and/or B cations. Although the

latter (i.e., fully removing A cations) is more frequently found in metal pnictides (e.g., skutterudites, $CoAs_3$),²⁰ the A cation site in HPs can be fully vacant, resulting in the so-called “A-site vacant BX_3 ” crystal structure, as is shown in Figure 2d. This type of structure is observed only in fluorides, like AlF_3 , FeF_3 , CoF_3 , and MnF_3 .⁵ Another variant of the ABX_3 perovskite is in the form of ordered perovskites (Figure 2e). Here, the B cations are heterovalently replaced by a combination of two (or more) cations that are located at specific crystallographic sites.²¹ In the case of HPs, this results in an A_2BCX_6 elpasolite structure (which is also sometimes termed “ $A_2BB'X_6$ ”), with its respective aristotype being the K_2NaAlF_6 mineral. Because of the double occupancy of the B-site cation, these perovskites are often simply called “double perovskites”, and they have been frequently studied as lead-free photovoltaic materials, albeit with limited success,²¹ or for broadband light emission.²² For heavy metal halides, the double perovskite subgroup includes materials such as $Cs_2AgInCl_6$, $Cs_2AgBiBr_6$, and MA_2AgSbI_6 , with a crystal structure that belongs to the $Fm\bar{3}m$ space group.²¹ It is important to note that these are not the same as mixed A, B, or X site perovskites (for example, $(Cs:MA:FA)-(Pb:Sn)(Br:I)_3$), in which the mixed cations occupying the respective A/B/X sites have the same valence, meaning that they do not occupy specific crystallographic sites. Furthermore, ordered perovskites have fixed stoichiometries, which is not the case for mixed perovskites. A variant of the double perovskite can also be obtained with a single metal in both the (I) and (III) oxidation states. These double perovskites include

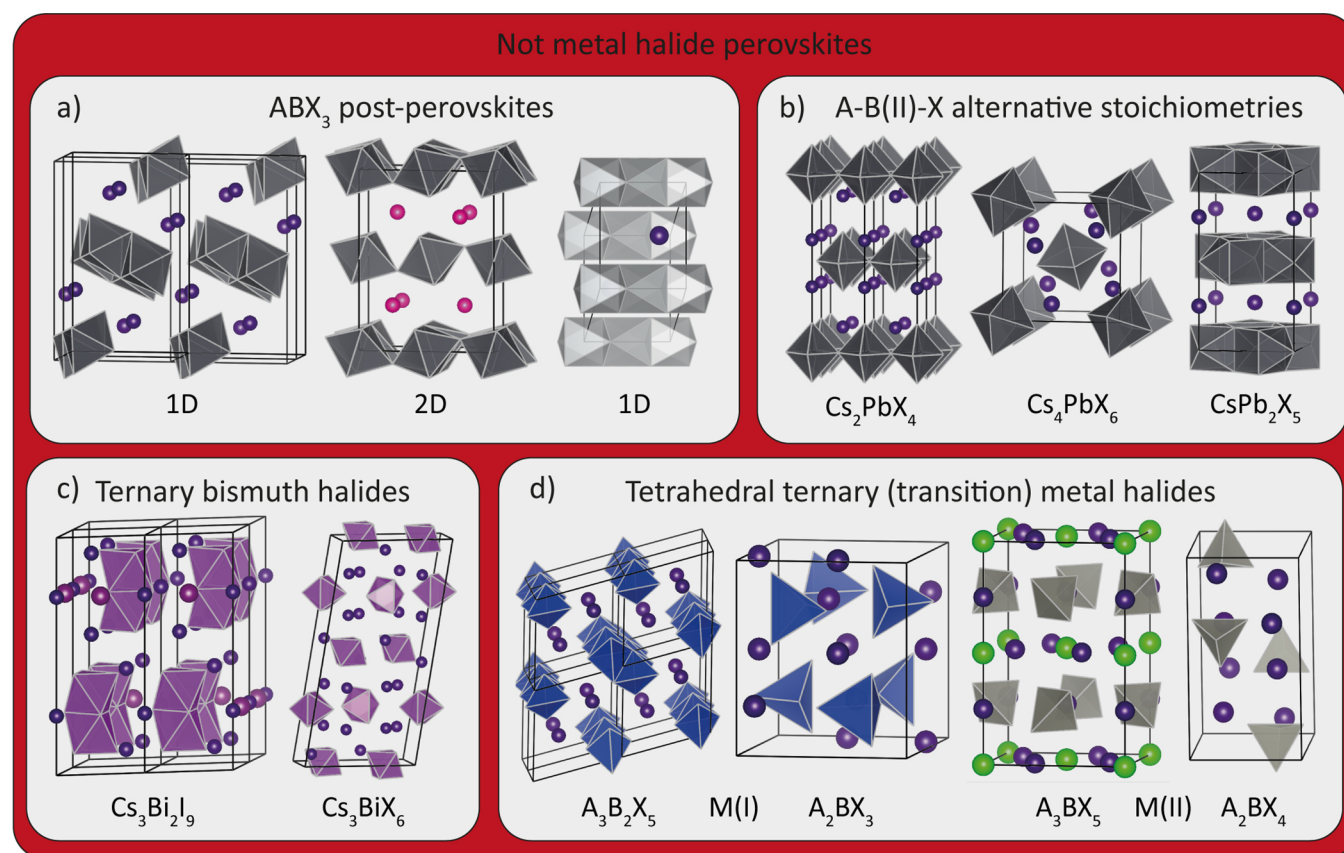


Figure 3. Overview of ternary metal halides not crystallizing in a perovskite structure. (a) Post-perovskites formed by ABX_3 ternary metal halides that would form stable perovskites at higher temperatures/pressures. (b) Ternary M(II) halides with nonperovskite stoichiometries, including inorganic Ruddlesden–Popper metal halide (A_2BX_4), A_4BX_6 , and AB_2X_5 phases. (c) Ternary bismuth halides not crystallizing in vacancy-ordered perovskites, including the isolated dimer structure ($Cs_3Bi_2I_9$) and isolated octahedra (Cs_3BiX_6). (d) Several ternary M(I) and M(II) (mainly transition metal and F^- and Cl^-) phases based on MX_4 tetrahedra.

materials such as $CsTiX_3$ and $CsAuX_3$ (even though the latter has strongly distorted octahedra).^{23,24} Finally, a small group of fluoride ordered perovskites crystallize in the A_3BX_6 cryolite (Na_3AlF_6) phase, where half of the B sites are occupied by the same cations that occupy the A sites (that is, the formula is the same as that of an ordered perovskite when it is written as A_2ABX_6).⁵ While the ordering of cations in HPs occurs only with B site cations, oxide perovskites can also form quadruple perovskites when both the A and B sites are occupied by two differently charged cations: these materials are generally described as having an $AA'BB'O_6$ formula, like $KSrXeNaO_6$, but the $CaCu_3Fe_2Re_2O_{12}$ compound also falls under this scheme.^{5,11,25} In the case of oxide perovskites, there are also examples of ordered perovskites that consist of either alternating layers or columns of different metal octahedra. One example of this type of ordered perovskites is $Sr_2La_2CuTi_3O_{12}$, which is formed by three layers of TiO_6 octahedra alternated with a layer of CuO_6 octahedra. These structures have not yet been reported for HPs, but any advances in this direction will certainly lead to interesting new halide materials.²⁶

The final subgroup of halide perovskites are vacancy-ordered perovskites (Figure 2f).²⁷ These are similar to ordered perovskites, but the B-site cation is partially replaced with a vacancy. Among the most studied vacancy-ordered perovskites are those belonging to the Cs_2BX_6 group, in which half of the B-site cations are occupied by M(IV) cations and the other half

by vacancies. Because these are crystallographically identical to ordered perovskites ($A_2B[V]X_6$, in which [V] is a vacancy), they share the same $Fm\bar{3}m$ space group. Vacancy-ordered perovskites in the M(IV) group include Cs_2SnI_6 , Cs_2PdBr_6 , Cs_2TeI_6 , and Cs_2TiBr_6 .²⁷ Vacancy-ordered perovskites can also form with trivalent metals like Sb^{3+} and Bi^{3+} . In this case, the B sites are not occupied by M(III) and by a vacancy in equal ratios; instead, they are occupied at a ratio of 2:1, resulting in an $A_3B_2X_9$ stoichiometry ($A_3B_2[V]X_9$) such as $Cs_3Sb_2I_9$.²⁸ In these ordered perovskites, the vacancies are ordered along the [111] planes, giving rise to a two-dimensional (2D) layer of BX_6 octahedra. By mixing these vacancy-ordered perovskites with Cd^{2+} , the fraction of vacancies can be further lowered to 25%, leading to a $Cs_4CdSb_2Cl_{12}$ ($A_4BC_2[V]X_{12}$) vacancy-ordered triple perovskite.²⁹ Because of the high concentration of vacancies, vacancy-ordered perovskites often exhibit low conductivity and thus have limited applications.²⁷ It is important to note that not all $A_3B_2X_9$ halides crystallize in this vacancy-ordered perovskite phase: for example, $Cs_3Bi_2I_9$ crystallizes in a nonperovskite phase (as will be discussed below).

Nonperovskite Inorganic Metal Halides. Not all ternary metal halides can form a stable perovskite structure. In general, the HP framework collapses if the A-site cation is either too small or too large for the metal halide network¹⁹ (the reader should refer to the Goldsmith tolerance factor, which is a figure of merit that indicates whether ternary metal halides can form

geometrically stable perovskites or not).^{12,30,31} As is shown in Figure 3a, ABX₃ metal halides that cannot form geometrically stable perovskites crystallize in either 1D or 2D edge-sharing octahedral lattices (like CsPbI₃ or RbPbBr₃, in which the A-site cation would be too small to stabilize the hypothetical perovskite structure) or a 1D face-sharing crystal lattice (like FAPbI₃, in which the A-site cation would be too large for the perovskite structure). The structural stability of ternary metal halide perovskites depends not only on the size of the ions but also on temperature and pressure:¹⁹ ternary metal halides that do not form stable perovskites under ambient conditions may do so at high temperatures or pressures; therefore, they are often called “post-perovskites”. In the case of LHPs, the two most studied post-perovskites are CsPbI₃ and FAPbI₃, both of which are post-perovskites under ambient conditions, but they form a perovskite phase when they are annealed at around 200–300 °C.¹⁹

Inorganic ternary M(II) halides (like those based on Sn²⁺ and Pb²⁺ ions) can also crystallize in several other stoichiometries (as shown in Figure 3b) with phases that can be very different from perovskites. One of these phases, the A₄BX₆ one (such as Cs₄PbBr₆), has often been called a “OD perovskite”.^{31,32} Although this phase consists of individual disconnected octahedra, similar to the A₂BX₆ vacancy-ordered perovskites, the BX₆ octahedra are no longer in the crystallographic positions that correspond to those of a perovskite. Moreover, the A-site cations now occupy two different crystallographic sites.³³ Therefore, an A₄BX₆ phase cannot be considered a perovskite. One ternary phase which is often called a “2D perovskite” is the AB₂X₅ phase (the most known example of which is CsPb₂Br₅). CsPb₂Br₅ is generally described as a stack of layers of connected [B₂X₅]⁺ clusters, separated by layers of Cs⁺ ions.³⁴ A close inspection of this structure (Figure 3b, right structure) reveals that it does not even contain MX₆ octahedra; therefore, it falls short of being considered a perovskite. Although thus not perovskites, these materials recently gained interest for their bright and narrow green photoluminescence (Cs₄PbBr₆ and CsPb₂Br₅) and for their use as a remote thermography material (Cs₂SnBr₆).^{31,32,35}

Heavy metal (Bi and Sb) based A₃B₂X₉ compounds usually crystallize in a vacancy-ordered perovskite structure (as mentioned above). However, ternary bismuth iodides with large A-site cations, like Cs₃Bi₂I₉, MA₃Bi₂I₉, and FA₃Bi₂I₉, crystallize in a different phase.³⁶ In this A₃B₂X₉ phase, [Bi₂I₉]³⁺ dimers are formed by two face-sharing BiI₆ octahedra, similar to Cs₃Cr₂Cl₉.³⁷ These dimers are separated by Cs⁺ ions, resulting in a hexagonal OD ternary metal halide, as is shown in Figure 3c. Thus, this phase does not much resemble a perovskite. Finally, Cs–Bi–X compounds can also crystallize in the Cs₃BiX₆ phase featuring single BX₆ octahedra which are no longer in the crystallographic positions that correspond to those of a perovskite. Therefore, they are not a A₃BX₆ cryolite, as described above. Consequently, they are not (double) perovskites.³⁸

In addition to the tolerance factor, another important parameter that dictates the stability of perovskites is the octahedral factor,¹² as it relates to the stability of the BX₆ octahedron. For instance, small cations that are coordinated by large anions (such as first row *d* metals and large anions like Br[−] and I[−]) generally prefer tetrahedral coordination. Therefore, HPs containing first row transition metals are primarily limited to fluorides, and there are only a few examples of HPs based on chlorides.¹² For example, ternary compounds like

A₃Cu₂X₅ and ACu₂X₃,³⁹ or compounds like A₂BX₄ and A₃BX₅ in which B is a first row transition metal (such as Zn²⁺, Ni²⁺, Cu²⁺, and Mn²⁺)⁴⁰ all consist of tetrahedral BX₄ clusters surrounded by A⁺ cations. Therefore, they cannot be classified as perovskites (see Figure 3d). However, they can be interesting nontoxic broad emitters (or at least less toxic than Pb-based ones).⁴⁰

Inorganic Layered Metal Halides. Among the various ternary metal halides, Ruddlesden–Popper (RP) phases (and layered metal halides in general, which will be discussed below) present a structurally interesting case. In the RP phase, which has an A₂BX₄ stoichiometry, a single 2D layer of corner-sharing M(II) halide octahedra is separated by a layer of A atoms (Figure 3b).⁴¹ Even though oxide RP phases can be synthesized using a wide variety of metals (such as Sr₂RuO₄, La₂NiO₄, and LaSrCoO₄),⁴² inorganic RP halide phases have, thus far, been limited to Cs₂PbI₂Cl₂ and Cs₂SnI₂Cl₂.⁴³ In an inorganic halide RP phase, the separation into layers is driven by the size difference between the two halides.⁴¹ Although (in oxides) these RP phases are often characterized as perovskites (“Ruddlesden–Popper perovskites”), it is our opinion that they should be classified only as RPs, and not as perovskites. We justify this opinion on the basis of the following two points: (i) These phases already have a common name (i.e., “Ruddlesden–Popper”). (ii) Starting from a perovskite structure, one cannot derive such phases without having to severely dismantle the perovskite lattice, at least locally. Furthermore, RP halides exhibit electronic and optical properties that are markedly different from their perovskite counterparts.⁴¹ The same reasoning applies to other phases consisting of stacks of layers made of corner-sharing octahedra, like Dion–Jacobson phases and the Aurivillius phase (both of which have been reported only for oxides to date),⁴⁴ as well as hybrid organic–inorganic layered metal halides, which will be discussed next.

Hybrid Organic–Inorganic Metal Halides. Hybrid organic–inorganic metal halides have gained an increasing amount of attention over the past decade.¹⁹ These are often also referred to as “hybrid perovskites” (Figure 4).^{9,45} In these materials, the A site is occupied by an organic cation, most commonly an alkyl ammonium cation. These types of materials are not organometallic compounds,^{46,47} as they do not contain any carbon–metal bonds, therefore they should not be called “organometallics” or “organolead” perovskites, but rather “hybrid organic–inorganic perovskites” (HOIPs).⁹ In the case of HOIPs, the A cations can consist of only small (pseudo spherical) MA and FA cations and the larger B cations, like Pb²⁺ and Sn²⁺,⁹ as is shown in Figure 4a. Here, it must be noted that not all of the hybrid organic–inorganic Pb and Sn halides form perovskites,¹⁹ as some (like FAPbI₃) are stable only at high temperatures, thus forming “post-perovskites” at ambient conditions.¹⁹ Small transition metal fluorides can also form stable HOIPs with NH₄⁺, like NH₄MnF₃ and NH₄ZnF₃.⁴⁸ Because of the anisotropy in the inorganic cations, the HOIPs have a lower symmetry than their inorganic counterparts, even in their pure cubic crystal structure.¹⁹ As the size of the A cation increases, layered compounds are formed, and these compounds usually crystallize in an A₂BX₄ (or ABX₄ in the case of cations with two ammonium groups) stoichiometry, in which layers of corner-sharing octahedra are separated by a layer of interlocking organic hydrocarbon chains (Figure 4c).^{45,49} Following the same line of reasoning as in the RP case above, these materials should not be considered

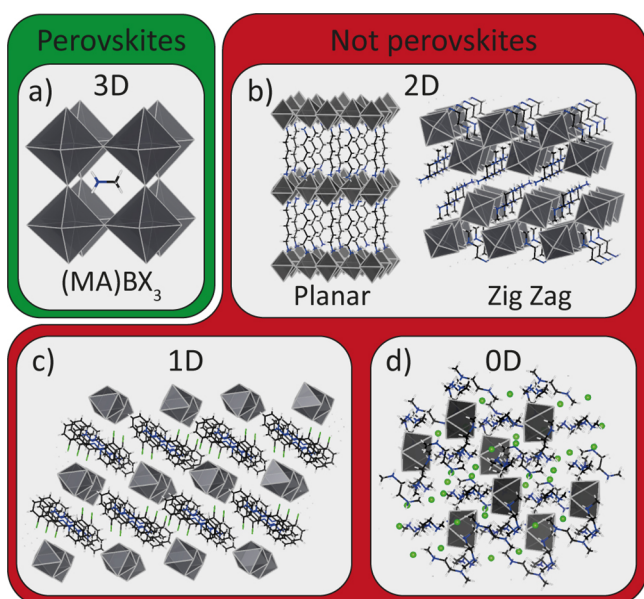


Figure 4. Overview of layered and hybrid organic–inorganic metal halides. (a) Hybrid organic–inorganic perovskite structure, with the A cation being a small organic cation like methylammonium. (b) Layered (2D) hybrid organic–inorganic metal halides, consisting of planar or zigzag corner-sharing octahedra. (c) 1D metal halides, consisting of chains of facet or corner-sharing octahedra. (d) 0D hybrid organic–inorganic metal halides, consisting of isolated metal halide octahedra.

perovskites either. In our opinion, these compounds should be simply classified as “layered hybrid organic–inorganic metal halides”.

One subclass of these layered hybrid organic–inorganic metal halides that has gained considerable interest because of their better moisture stability and higher degree of optoelectronic fine-tuning than conventional lead halide perovskites is the one containing several consecutive layers of 3D connected metal halides alternated with a single layer of organic cations (often called “2D perovskites” or “layered perovskites”).¹⁹ These compounds can be synthesized by using a mixture of a small cation that can form a perovskite (e.g., Cs^+ or MA) and a large organic cation that can form only layered metal halides. These layered materials have a general $[L]A_{n-1}B_nX_{3n+1}$ formula, in which L is the large organic cation (sometimes referred to as a “ligand”) and n is the number of layers of 3D connected octahedra.^{45,46,49} In this case, the line

between a layered metal halide ($n = 1$) and a perovskite ($n \approx \infty$) remains a topic of debate and, to a certain extent, a matter of opinion. Finally, hybrid organic–inorganic metal halides have been reported using bulky organic cations or organic cations consisting of multiple ammonium groups.⁴⁶ These compounds often are either formed by single chains of metal halide octahedra (Figure 4c) or by completely isolated metal halide clusters (Figure 4d), and they are sometimes referred to as “1D” or “0D organic perovskites”.⁴⁶ These types of compounds have very little in common with the perovskite crystal structure, therefore they should not be identified as perovskites, but rather as “0D” or “1D hybrid organic–inorganic metal halides”.

Antiperovskite with Halide B Sites. Although the aforementioned AB_2X_5 and A_3BX_5 compositions do not consist of octahedrally coordinated metal cations (and are therefore strictly not perovskites), they can qualify as inverse antiperovskites, because they have XB_6 octahedra and small X or BX clusters occupying the A site. They are not the same as antiperovskites, in which the halides generally occupy only the A site, and are not part of the perovskite framework. In the case of an A_3BX_5 phase, using Cs_3ZnBr_5 as an example, the Br^- anion can be interpreted as being octahedrally coordinated by Cs^+ cations, resulting in a $[BrCs_6]^{2+}$ cubic framework.⁵⁰ Within this framework, the $[ZnBr_4]^{2-}$ clusters occupy the A sites, as is shown in Figure 5a. This is also similar to a double antiperovskite $Na_6FeCl(SO_4)_2$ (sulphohalite, a natural mineral), in which the A site is occupied by a SO_4^{2-} cluster and the perovskite framework consists of FNa_6 and $ClNa_6$ octahedra, as well as $Ba_3(FeS_4)Br$, which has a $[FeS_4]^{-5}$ A-site cluster.^{5,51} Small inorganic clusters in A sites can also be found in a standard perovskite structure, like Tl_4SnTe_3 , which is a chalcogenide perovskite (consisting of $SnTe_6$ octahedra) with an A site that is occupied by a tetrahedral Tl_4^{4+} cluster.⁵² Similarly, the AB_2X_5 phase (for example, $CsPb_2Br_5$, as is shown in Figure 5b) can also be considered an antiperovskite consisting of octahedrally coordinated halide anions. Here, $[BrPb_4Cs]^{4+}$ octahedra form a perovskite framework, with the A cation site being occupied by a cluster of 4 Br^- ions. This is analogous to the $TlSn_2I_5$ case.⁵³ The possibility for small inorganic clusters to occupy the A site of a standard perovskite was recently demonstrated with the vacancy-ordered halide perovskite structure of $Cs_3Cu_4In_2Cl_{13}$, in which 25% of the A sites are occupied by $[Cu_4Cl]^{3+}$ clusters and half of the B sites are vacant (a structure that can be more appropriately described as $([Cu_4Cl]Cs_3In_2[V]_2Cl_{12})$, is shown in Figure 5c.⁵⁴ These cases of inverse antiperovskites, together with the

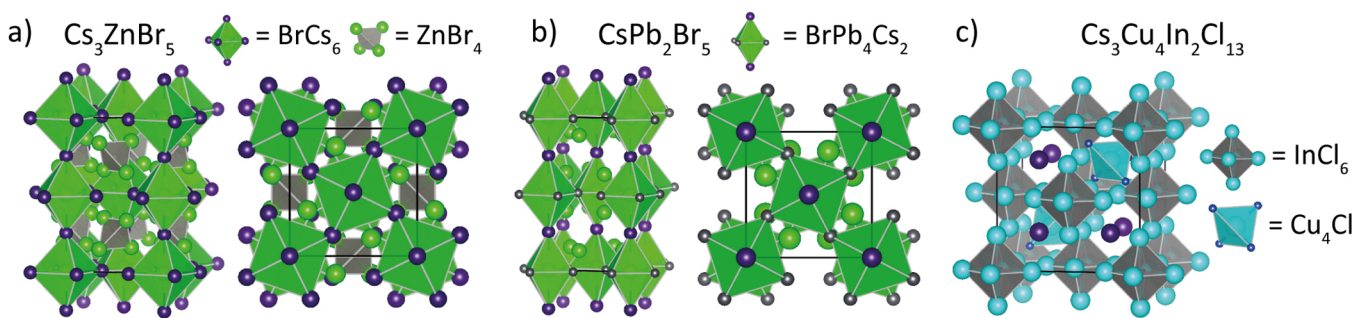


Figure 5. Antiperovskites of A_3BX_5 and AB_2X_5 phases. (a) Cs_3ZnBr_5 and (b) $CsPb_2Br_5$ with (left) polyhedra centered on the halides and (right) top view shown along the c -axis. (c) $Cs_3Cu_4In_2Cl_{13}$ vacancy-ordered perovskite, consisting of $InCl_6^{3-}$ octahedra and Cu_4Cl^{3+} tetrahedra occupying the A sites.

inverse perovskites like BaLiF_3 , demonstrate that the A-site cations in perovskites are not simply limited to alkali metals (or small organic molecules), but they can also consist of small inorganic clusters and metal cations with different charges, a consideration that should inspire the discovery of new halide perovskites.

Conclusions and Recommendations. Although there are many different types of HPs, the recent and rapid advancements in the field has led to a confusion on the correct way of naming all the different compounds that have been reported. In our opinion, if a compound is to be considered a “perovskite”, it must have an ABX_3 (or equivalent) stoichiometry consisting of a cubic network of corner-sharing BX octahedra, with the following exceptions: (i) the A and B sites can be partially or fully vacant or ordered; (ii) the A cations can consist of small organic molecules or inorganic clusters; (iii) the formation of anti-halide perovskites, with a halide occupying either the A or B site. 1D and 0D hybrid organic–inorganic metal halides do not satisfy these conditions; therefore, they should not be considered as perovskites. Although this is a somewhat controversial subject, layered Ruddlesden–Popper (and similar) phases, as well as 2D hybrid organic–inorganic metal halides, do not fit these criteria either. Thus, it is our opinion that they should not be referred to as perovskites. As a final comment, we stress the importance of stating whether a perovskite is vacant, ordered, anti, or a combination of these. This not only identifies the deviations from a typical perovskite stoichiometry but also, in most cases, explains the completely different properties of the materials compared to their perovskite equivalent.

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Notes

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