The role of nonmagnetic $d^0$ vs. $d^{10}$ $B$-type cations on the magnetic exchange interactions in osmium double perovskites

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Polycrystalline samples of double perovskites Ba$_2$BOsO$_6$ ($B =$ Sc, Y, In) were synthesized by solid state reactions. They adopt the cubic double perovskite structures (space group, \textit{Fm}$-\textit{3m}$) with ordered $B$ and Os arrangements. Ba$_2$BOsO$_6$ ($B =$ Sc, Y, In) show antiferromagnetic transitions at 93 K, 69 K, and 28 K, respectively. The Weiss-temperatures are -590 K for Ba$_2$ScOsO$_6$, -571 K for Ba$_2$YOsO$_6$, and -155 K for Ba$_2$InOsO$_6$. Sc$^{3+}$ and Y$^{3+}$ have the open-shell $d^0$ electronic configuration, while In$^{3+}$ has the closed-shell $d^{10}$. This indicates that a $d^0$ $B$-type cation induces stronger overall magnetic exchange interactions in comparison to a $d^{10}$. Comparison of Ba$_2$BOsO$_6$ ($B =$ Sc, Y, In) to their Sr and Ca analogues shows that the structural distortions weaken the overall magnetic exchange interactions.

\textbf{Keywords:} Osmium; double perovskite; magnetic exchange interaction; structural distortion.
Introduction

Double perovskite oxides, $A_2BB'O_6$, containing 4d/5d elements have attracted considerable attention due to their remarkable electronic and magnetic properties, such as room-temperature magnetoresistance [1], high-temperature ferrimagnetism [2,3], as well as spin glass [4] and valence bond glass behaviors[5]. As a characteristic structural feature, there are interpenetrating $B$ and $B'$ face-centered cubic (fcc) sublattices, and their complex magnetic properties are determined by the intricate interplay between the geometrically frustrated intra-sublattice and inter-sublattices exchange interactions, which are correlated with structure distortions [6-11]. The well-studied isoelectronic double perovskites Sr$_2$FeOsO$_6$ [12-15], and Ca$_2$FeOsO$_6$ [3,7] are exemplary. Sr$_2$FeOsO$_6$ crystallizes in a tetragonal double perovskite structure (space group: I4/m) and shows successive antiferromagnetic (AFM) transitions around 140 K and 67 K [12,13], while the isoelectronic Ca$_2$FeOsO$_6$ crystallizes in a monoclinic variant (space group: $P2_1/n$) and shows room temperature ferrimagnetism [3,7].

When in $A_2BB'O_6$ $B$ is a nonmagnetic cation and $B'$ is Os$^{5+}$, the magnetic properties are obviously determined by exchange coupling within the Os$^{5+}$ fcc sublattice. Investigations into double perovskites with single Os$^{5+}$ magnetic sublattice will provide help for a better understanding of the remarkable magnetic properties of osmium double perovskites, such as the exceptionally high-temperature ferrimagnetism in Sr$_2$CrOsO$_6$ [2] and the strikingly different magnetic properties between Sr$_2$FeOsO$_6$ [12,13] and Ca$_2$FeOsO$_6$ [3,7]. Most of the well-studied double perovskites with nonmagnetic $B$ cations and Os$^{5+}$ forming the $B'$ sublattice known so far display AFM transitions [16-23]. Because the magnetic interactions between the nearest-neighbor (NN) Os$^{5+}$ ions are usually thought to run mainly via the Os$^{5+}$-O-O-Os$^{5+}$ path [16,17,20,22], the nonmagnetic $B$ cations are not expected to play an important role in the magnetic exchange interactions. However, investigations on Sr$_2$BOsO$_6$ ($B$ = Sc, Y, In) indicate that the electronic configuration of the nonmagnetic $B$ cation, d$^0$ or d$^{10}$, does influence the magnetic exchange interactions [16,24]. As Sr$_2$BOsO$_6$ ($B$ = Sc, Y, In) are also structurally distorted, but to a different degree [16], it is better to study the role of nonmagnetic $B$ cations in distortion-free analogues. As a simple measure, substituting Ba for Sr would yield cubic double perovskites. In this work, undistorted double perovskites Ba$_2$ScOsO$_6$, Ba$_2$YOso$_6$, and Ba$_2$InOsO$_6$ were synthesized and their magnetic properties were characterized. By comparing their magnetic properties, we were able to address the role of nonmagnetic d$^0$ vs. d$^{10}$ cations on the magnetic exchange interactions. We have also compared their structural and magnetic properties to those of the Sr and Ca analogues, thereby obtaining information on the effects of structural distortions on the magnetic exchange interactions. The synthesis of Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$ was
firstly reported by Slight et al. [25]; however, to the best of our knowledge, details of their magnetic properties are not known to date. The synthesis and magnetic properties of Ba$_2$YO$_6$O$_6$ were published by Kermarrec et al. [23].

**Experimental**

Polycrystalline samples of Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$ were synthesized by the solid-state reaction from powders of BaO$_2$ (Alfa Aesar, anhydrous, 84% min), Sc$_2$O$_3$ (Alfa Aesar, 99.9%)/In$_2$O$_3$ (Alfa Aesar, 99.99%), and OsO$_2$ (Alfa Aesar, 83% Os min). BaO$_2$, B$_2$O$_3$ ($B =$ Sc or In), and OsO$_2$ were weighted with mole ratio 4:1:2, thoroughly mixed, and pressed into pellets inside a glove box. Then the pellets were transferred into corundum crucibles, which were placed and sealed inside quartz ampules. Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$ were obtained after sintering for 96 hours at 1025 ºC and 950 ºC, respectively, with once intermittent regrinding. A polycrystalline sample of Ba$_2$YO$_6$O$_6$ was synthesized by solid-state reaction from powders of BaO$_2$ (99%, Kojundo Chemical Lab. Co., Ltd.), Os (99.95%, Heraeus Materials Technology), Y$_2$O$_3$ (99.99%, Kojundo Chemical Lab. Co., Ltd.), and KClO$_4$ (>99.5%, Kishida Chemical Co., Ltd.). The starting materials with stoichiometric ratio were weighted and thoroughly mixed, followed by sealing in a Pt capsule. The sealed Pt capsule was then statically compressed in a belt-type high-pressure apparatus at a pressure of 6 GPa, followed by heating at 1500 ºC for 1 hour, while maintaining the high-pressure conditions. It was then quenched to ambient temperature in less than a minute, and subsequently, the pressure was released.

Small pieces of Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$ were cut from the synthesized pellets and finely ground for powder X-ray diffraction (Guinier technique, Huber G670 camera. Cu-K$_\alpha 1$ radiation, $\lambda =$ 1.54056 Å, germanium monochromator, $10^\circ \leq 20 \geq 100^\circ$, step width of 0.005°). A small piece of Ba$_2$YO$_6$O$_6$ was finely ground and rinsed in water to remove any KCl residue. The final black powder was investigated by synchrotron X-ray diffraction (SXRD), which was conducted using a large Debye–Scherrer camera installed in the BL15XU beamline in SPring–8. The SXRD data were collected at $\lambda =$ 0.65298 Å (confirmed by a reference material, CeO$_2$) at room temperature. The refinement of crystal structures was carried out by Rietveld analysis using the RIETAN-VENUS software [26,27].

Using pieces of the obtained pellets, the electrical resistivities ($\rho$) were measured with a DC gauge current of 0.1 mA by a four-point method using a physical properties measurement system (PPMS, Quantum Design, Inc.). Electrical contacts were made with Au wires and silver paste. The temperature dependence of the specific heat ($C_p$) was measured in the same PPMS apparatus by using its HC option (relaxation method). The magnetic susceptibilities ($\chi$) of the samples were
measured in a SQUID magnetometer (MPMS, Quantum Design), at field cooling (FC) conditions in a temperature range between 2 K and 380 K under applied magnetic fields of 10 kOe for Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$, but 70 kOe for Ba$_2$YOsO$_6$.

**Results and discussions**

Figure 1. Rietveld refined powder XRD profiles of Ba$_2$ScOsO$_6$ (top) and Ba$_2$InOsO$_6$ (middle) and rietveld refined powder SXRD profile of Ba$_2$YOsO$_6$ (bottom); the insets show the corresponding crystal structures.

The room temperature XRD patterns of Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$ and the SXRD pattern of Ba$_2$YOsO$_6$ are shown in Figure 1. They are well refined assuming cubic double perovskite structures with space group *Fm*-3*m*. The obtained lattice parameters are $a = 8.15249(4)$ Å for Ba$_2$ScOsO$_6$, $a = 8.22424(4)$ Å for Ba$_2$InOsO$_6$, and $a = 8.35131(1)$ for Ba$_2$YOsO$_6$, which are almost as same as those reported, 8.152 Å for Ba$_2$ScOsO$_6$, 8.224 Å for Ba$_2$InOsO$_6$, and $a = 8.3541(4)$ for Ba$_2$YOsO$_6$ [24,25]. The XRD or SXRD pattern of Ba$_2$ScOsO$_6$ and Ba$_2$YOsO$_6$, respectively, indicates that the sample is free from impurities. However, in the XRD pattern of Ba$_2$InOsO$_6$, in addition to
the Bragg reflections expected for Ba$_2$InOsO$_6$, several weak reflections were could be observed, which can be attributed to In$_2$O$_3$ impurity (about 1% wt). The impurity is diamagnetic and thus does not have any impact on the magnetic properties. During the analysis, the possible anti-site disorder between $B$ and Os was carefully checked under the conditions that he 4$a$ and 4$b$ Wyckoff site are constrained to be fully occupied and the mole ratio $B$/Os were constrained to be 1/1. The occupancies of $B$ and Os were then refined with fixed displacement parameters of 0.5. In subsequent cycles the displacement parameters were refined while the occupancies were fixed. This procedure was repeated several times, while the scale factor, peak-shape parameters, asymmetry parameters, lattice parameters and atomic position parameters were refined during the analysis. The obtained atomic positions, occupancy, and isotropic displacement parameters for Ba$_2$BOSO$_6$ ($B = \text{Sc, Y, In}$) at room temperature are shown in Table 1. Within the error limits, the results of the analysis indicated a 100% order of Y and Os, but small amount of disorder of Sc/In and Os. Investigations on crystal structures of ordered double perovskites $A_2M^{3+}$TaO$_6$ and $A_2M^{3+}$NbO$_6$ reveal that the compounds showing 100% $B/B'$ order usually have large ionic radius difference ($\Delta r \geq 0.26$ Å) between $B$ and $B'$ ions [28]. In this work, the $\Delta r$ for Ba$_2$BOSO$_6$ ($B = \text{Sc, Y, In}$) are 0.17, 0.325, and 0.225 Å, respectively [29], which is consistent with the findings in Ref. 28.

Table 1. Atomic positions, occupancy, and isotropic displacement parameters for Ba$_2$BOSO$_6$ ($B = \text{Sc, Y, In}$) at room temperature.

| Compounds       | Atoms      | Site | Occupancy | x    | y    | z    | $B_{iso}$ (Å$^2$) |
|-----------------|------------|------|-----------|------|------|------|-------------------|
| Ba$_2$ScOsO$_6$ | Ba 8$c$    | 1    | 0.25      | 0.25 | 0.25 | 0.28(2)          |
|                 | Sc1/Os1 4$a$ | 0.98(1)/0.02 | 0     | 0    | 0    | 0.20(2)          |
|                 | Os2/Sc2 4$b$ | 0.98/0.02 | 0.5   | 0    | 0    | 0.19(2)          |
|                 | O 24$e$    | 1    | 0.2618(3) | 0    | 0    | 0.16(6)          |
| Ba$_2$YOsoO$_6$ | Ba 8$c$    | 1    | 0.25      | 0.25 | 0.25 | 0.50(1)          |
|                 | Y 4$a$     | 1    | 0     | 0    | 0    | 0.24(2)          |
|                 | Os 4$b$    | 1    | 0.5   | 0    | 0    | 0.26(1)          |
|                 | O 24$e$    | 1    | 0.2669(3) | 0    | 0    | 0.49(5)          |
| Ba$_2$InOsO$_6$ | Ba 8$c$    | 1    | 0.25      | 0.25 | 0.25 | 0.24(3)          |
|                 | In1/Os1 4$a$ | 0.97(1)/0.03 | 0     | 0    | 0    | 0.43(4)          |
|                 | Os2/In2 4$b$ | 0.97/0.03 | 0.5   | 0    | 0    | 0.43(3)          |
|                 | O 24$e$    | 1    | 0.2624(7) | 0    | 0    | 0.34(8)          |
Figure 2. Temperature dependent magnetic susceptibilities of Ba$_2$ScOsO$_6$ (top), Ba$_2$YOsO$_6$ (middle), and Ba$_2$InOsO$_6$ (bottom). Insets show the corresponding plots of their inverse susceptibilities.
The temperature dependent magnetic susceptibilities, $\chi(T)$, of Ba$_2$ScOsO$_6$, Ba$_2$YOsO$_6$, and Ba$_2$InOsO$_6$ are shown in Figure 2. Ba$_2$ScOsO$_6$, Ba$_2$YOsO$_6$, and Ba$_2$InOsO$_6$ show a maximum at temperatures of 93 K, 69 K, and 28 K, respectively, indicating the onset of AFM ordering. In comparison to Ba$_2$InOsO$_6$, the curvature of $\chi(T)$ for Ba$_2$ScOsO$_6$ and Ba$_2$YOsO$_6$ is concave upon approach to Néel temperature ($T_N$), suggesting the presence of short range magnetic correlations. To further characterize these magnetic transitions, specific heat was measured (see Figure 3). Lambda-type anomalies can be observed around temperatures of 93 K, 69 K, and 28 K for Ba$_2$ScOsO$_6$, Ba$_2$YOsO$_6$, and Ba$_2$InOsO$_6$, respectively, confirming the formation of long range AFM order.

![Figure 3. Temperature dependence of the specific heat of Ba$_2$ScOsO$_6$ (top), Ba$_2$YOsO$_6$ (middle), and Ba$_2$InOsO$_6$ (bottom).](image)

Curie-Weiss analysis of the high-temperature part of the inverse susceptibility has resulted in the effective moment, $\mu_{\text{eff}}$, of 3.26 $\mu_B$ for Ba$_2$ScOsO$_6$, 3.45 $\mu_B$ for Ba$_2$YOsO$_6$, and 2.89 $\mu_B$ for
Ba$_2$InOsO$_6$. The extracted Weiss-temperatures, $\Theta_W$, are -590 K for Ba$_2$ScOsO$_6$, -538 K for Ba$_2$YOsO$_6$, and -181 K for Ba$_2$InOsO$_6$. These $\mu_{\text{eff}}$ values are comparable with most of the values reported for Os$^{5+}$, in the range of 2.71-3.72 $\mu_B$ [16-22,30], but they are lower than the theoretical spin-only moment (3.87 $\mu_B$) for Os$^{5+}$ ($S = 3/2$), which can be partially attributed to the reduction of Os$^{5+}$ $\mu_{\text{eff}}$ due to spin-orbit coupling. It has been suggested that the effect of spin-orbit coupling cannot be ignored in 4d$^3$ and 5d$^3$ systems [31].

The negative $\Theta_W$ reflects that AFM correlations are predominant in these compounds. Ba$_2$ScOsO$_6$ and Ba$_2$InOsO$_6$ are electrically semiconducting (see Figure 4), similar to other double perovskites with single Os$^{5+}$ magnetic sublattices [16-22]. Attempts were made to plot the data on a $T^{1/4}$ scale, and both samples are found to be linear on a $T^{1/4}$ scale as shown in the inset of Figure 4, in accordance with a three-dimensional variable range hopping transport model. Their magnetic exchange interactions should be dictated by extended superexchange interactions such as Os$^{5+}$-O-O-Os$^{5+}$. The large negative $\Theta_W$ of -590 K for Ba$_2$ScOsO$_6$ and -538 K for Ba$_2$YOsO$_6$ indicate very strong AFM exchange interactions. Strikingly, the $\Theta_W$ for Ba$_2$InOsO$_6$ is only -181 K. Because they all crystallize in the same cubic double perovskite structure, the difference among Ba$_2$BOsO$_6$ ($B$ = Sc, Y, In) is that they have different nonmagnetic $B$-type cations. Sc$^{3+}$ and Y$^{3+}$ have the open-shell 3d$^0$ and 4d$^0$ electronic configurations, respectively, but In$^{3+}$ has the closed-shell 4d$^{10}$ electronic configuration. The large change of $\Theta_W$ from -538 K and -590 K for Ba$_2$ScOsO$_6$ and Ba$_2$YOsO$_6$, respectively, to -181 K for Ba$_2$InOsO$_6$ indicates that a d$^0$ $B$-type cation induces stronger overall magnetic exchange interactions in comparison to a d$^{10}$ $B$-type cation. Here we note that in our undistorted cubic double perovskites, an s or p orbital at the $B$-type cation cannot mediate the NN Os$^{5+}$-O-$B$-O-Os$^{5+}$ exchange interaction (Os$^{5+}$-$t_{2g}^3$, Os$^{5+}$-$B$-Os$^{5+}$-90º bond angle) so that the difference between the Sc/Y vs the In compounds must be attributed to the difference in the d-configuration. Indeed, the first-principles density functional theory studies of Sr$_2$BOsO$_6$ ($B$ = Sc, Y, In) reveal that the electronic configuration of nonmagnetic $B$ cations, either open shell d$^0$ or closed shell d$^{10}$, has an increasing or decreasing influence on the hybridization between the Os-5d and Sc/Y/In-d states, and it was found that the exchange coupling depends strongly on the overlap between Os-5d and Sc/Y/In-d states [24]. The hybridization between Os-5d and Sc/Y/In-d states is much smaller in the d$^{10}$ closed-shell case than in the d$^0$ open-shell cases, which results in the smaller amplitudes of Os-Os coupling in the In$^{3+}$ compound than in the Y$^{3+}$ and Sc$^{3+}$ compounds [24].
In double perovskites $\text{Ba}_2\text{BO}_6$ ($B = \text{Sc}, \text{Y}, \text{In}$), Os$^{5+}$ ions form fcc sublattices, and they are magnetically frustrated when the AFM NN Os$^{5+}$-Os$^{5+}$ interactions are predominant. The $T_N$s of $\text{Ba}_2\text{BO}_6$ ($B = \text{Sc}, \text{Y}, \text{In}$) are 93 K, 69 K, and 28 K, respectively, which are much lower than their $|\Theta_W|$ values, clearly indicating the presence of magnetic frustration. The frustration factor, $|\Theta_W/T_N|$, is 6.3, 7.8, and 6.5 for $\text{Ba}_2\text{ScOsO}_6$, $\text{Ba}_2\text{YOsO}_6$, and $\text{Ba}_2\text{InOsO}_6$, respectively. $\text{Ba}_2\text{YOsO}_6$ was reported to adopt the type-I fcc spin structure [23]. In type-I spin structure, each osmium is antiferromagnetically coupled to eight out of twelve NN ions, but the NNN ions are all ferromagnetically coupled. It is usually stabilized when the AFM NN interactions are predominant, whereas the next-nearest-neighbor interactions are either ferromagnetic or negligibly small [32]. Because $\text{Ba}_2\text{BO}_6$ ($B = \text{Sc}, \text{Y}, \text{In}$) are magnetic frustrated and have comparable values of $|\Theta_W/T_N|$, $\text{Ba}_2\text{ScOsO}_6$ and $\text{Ba}_2\text{InOsO}_6$ may adopt the same type-I spin structures as $\text{Ba}_2\text{YOsO}_6$. The similar compounds $\text{Sr}_2\text{BO}_6$ ($B = \text{Sc}, \text{Y}, \text{In}$) were reported to adopt type-I spin structures [16,17]. Further neutron diffraction and theoretical calculation are needed for the determination of magnetic structures of $\text{Ba}_2\text{ScOsO}_6$ and $\text{Ba}_2\text{InOsO}_6$.

The space groups, lattice parameters, average bond angles of $\text{B-O-Os}$, and magnetic properties of double perovskites $\text{Ba}_2\text{BO}_6$ ($B = \text{Sc}, \text{Y}, \text{In}$) and their Sr and Ca analogues are summarized in Table 2. $\text{Ba}_2\text{BO}_6$ ($B = \text{Sc}, \text{Y}, \text{In}$) crystallize in the ideal double perovskite structures, in which there is no structural distortion and the $\text{B-O-Os}$ bond angles are 180º. When Ba$^{2+}$ is replaced
by the smaller cation $\text{Sr}^{2+}$, the crystal structures distort and the $B$-$O$-$\text{Os}$ bond angles deviate from $180^\circ$ in order to accommodate the smaller $A$ site cation. When $\text{Sr}^{2+}$ is replaced by the even smaller cation $\text{Ca}^{2+}$, the crystal structures are even more distorted with more buckled $B$-$O$-$\text{Os}$ bonds.

Generally, the values of $|\Theta_W|$ for $\text{Ba}_2\text{BO}_6\text{OsO}_6$ ($B = \text{Sc, Y, In}$) are larger than those of their $\text{Sr}$ and $\text{Ca}$ analogues, suggesting that the strength of the overall Os$^{5+}$-Os$^{5+}$ magnetic exchange interactions correlates negatively with structural distortions: the structural distortions weaken the overall magnetic exchange interactions. All these double perovskites with single Os$^{5+}$ magnetic sublattice display long range AFM order and show magnetic frustration as indicated by an average $|\Theta_W/T_N|$ value of $\approx 6.5$. Apparently, there is no clear correlation between the $|\Theta_W/T_N|$ and the structural distortions.
Table 2. Double perovskites with single Os$^{5+}$ magnetic sublattice.

| Compound $A_2BO$Os$^{5+}$O$_6$ | Space group | Lattice parameters (Å or ° or Å$^3$) | Average $\angle B-O$-Os (°) | $T_N$ (K) | $\Theta_W$ (K) | $\mu_{\text{eff}}$ ($\mu_B$) | $|\Theta_W/T_N|$ | Ref. |
|--------------------------------|-------------|--------------------------------------|-------------------------------|-------------|----------------|-----------------|----------------|------|
| Ca$_2$ScOsO$_6$ P2$_1/n$       | a = 5.4716(1) b = 5.6165(1) c = 7.8168(1) $\beta$ = 89.889(2) V/Z = 120.109  | 151.3  | 69   | -341 | 3.72 | 4.9 | [22] |
| Sr$_2$ScOsO$_6$ P2$_1/n$       | a = 5.6666(1) b = 5.6428(1) c = 7.9791(1) $\beta$ = 90.083(2) V/Z = 127.620  | 166.1  | 92   | -606 | 2.99 | 6.5 | [16] |
| Ba$_2$ScOsO$_6$ Fm-3m          | a = 8.15249(4) V/Z = 135.460  | 180   | 93   | -590 | 3.26 | 6.3 | this work |
| Sr$_2$YOsO$_6$ P2$_1/n$        | a = 5.7817(1) b = 5.8018(1) c = 8.1877(1) $\beta$ = 90.227(1) V/Z = 136.945  | 157.3  | 53   | -337 | 3.45 | 6.4 | [16] |
| Ba$_2$YOsO$_6$ Fm-3m           | a = 8.3541(4) V = 145.760  | 180   | 67.69 | -717 | 3.93 | 10.4 | [23] |
|                               | a = 8.35131(1) V/Z = 145.614  | 180   | 69   | -571 | 3.52 | 8.3 | this work |
| Ca$_2$InOsO$_6$ P2$_1/n$       | a = 5.4889(3) b = 5.6785(1) c = 7.8576(2) $\beta$ = 90.12(2) V/Z = 122.456  | 147.4  | 14   | -77  | 3.15 | 5.5 | [18] |
| Sr$_2$InOsO$_6$ P2$_1/n$       | a = 5.7002(1) b = 5.6935(1) c = 8.0521(1) $\beta$ = 90.112(1) V/Z = 130.695  | 158.5  | 26   | -103 | 3.08 | 4.0 | [16] |
| Ba$_2$InOsO$_6$ Fm-3m          | a = 8.22424(4) V/Z = 139.068  | 180   | 28   | -155 | 2.84 | 5.5 | this work |
Conclusions

Polycrystalline samples of Ba$_2$BOsO$_6$ ($B = \text{Sc, Y, In}$) were synthesized by solid state reactions. Their structural and magnetic properties were investigated. Room temperature XRD showed that they all crystallize as ordered double perovskites with space group $Fm-3m$. Magnetic susceptibilities and specific heat measurements revealed that Ba$_2$BOsO$_6$ ($B = \text{Sc, Y, In}$) order antiferromagnetically at 93 K, 69 K, and 28 K, respectively. The extracted $\Theta_W$ is -590 K for Ba$_2$ScOsO$_6$, -571 K for Ba$_2$YOso$_6$, and -155 K for Ba$_2$InOsO$_6$. Sc$^{3+}$ and Y$^{3+}$ have the open-shell d$^0$ electronic configurations, but In$^{3+}$ has the closed-shell d$^{10}$ electronic configuration, indicating that a d$^0$ B-type cation induces stronger overall AFM exchange interactions in comparison to a d$^{10}$ B-type cation. Comparison of Ba$_2$BOsO$_6$ ($B = \text{Sc, Y, In}$) to the Sr and Ca analogues showed that the structural distortions weaken the overall AFM exchange interactions.

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