Coupled magnetic and structural phase transitions in antiferromagnetic polar metal Pb$_2$CoOsO$_6$ under pressure

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Abstract

Pb$_2$CoOsO$_6$ is a newly synthesized polar metal in which inversion symmetry is broken by the magnetic frustration in an antiferromagnetic ordering of Co and Os sublattices. The coupled magnetic and structural transition occurs at 45 K at ambient pressure. Here we perform transport measurements and first-principles calculations to study the pressure effects on the magnetic/structural coupled transition of Pb$_2$CoOsO$_6$. Experimentally we monitor the resistivity anomaly at $T_N$ under various pressures up to 11 GPa in a cubic anvil cell apparatus. We find that $T_N$ determined from the resistivity anomaly first increases quickly with pressure in a large slope of $dT_N/dP = +6.8(8)$ K/GPa for $P < 4$ GPa, and then increases with a much reduced slope of 1.8(4) K/GPa above 4 GPa. Our first-principles calculations suggest that the observed discontinuity of $dT_N/dP$ around 4 GPa may be attributed to the vanishing of Os magnetic moment under pressure. Pressure substantially reduces the Os moment and completely suppresses it above a critical value, which relieves the magnetic frustration in the antiferromagnetic ordering of Pb$_2$CoOsO$_6$. The Co and Os polar distortions decrease with the increasing pressure and simultaneously vanish at the critical pressure. Therefore above the critical pressure a new centrosymmetric antiferromagnetic state emerges in Pb$_2$CoOsO$_6$, distinct from the one under ambient pressure, thus showing a discontinuity in $dT_N/dP$.

Keywords: Pb$_2$CoOsO$_6$, polar metal, pressure effect, antiferromagnetism
I. INTRODUCTION

Ferroelectricity is usually incompatible with long-range magnetic order and metallicity\textsuperscript{1–3}. Insulating materials which possess both electric polarization and magnetization and possibly a coupling between the two order parameters are called multiferroics, which has been an active research field in condensed matter physics and materials science\textsuperscript{4–6}. On the other hand, materials with both polar displacements and intrinsic metallicity are termed as “polar metals”\textsuperscript{3,7}, which have attracted increasing interest in experiment and theory\textsuperscript{8–17}. According to Anderson and Blount\textsuperscript{3}, polar metals are characterized by a second-order structural phase transition with the appearance of a polar axis and the loss of inversion symmetry at a finite temperature. \textit{LiOsO}_3 is the first unambiguous example of bulk polar metals, which transforms from a centrosymmetric \textit{R¯3c} structure to a polar \textit{R3c} structure at \(T_s = 140\) K\textsuperscript{7,18}. However, a \textit{metal} that possesses both polar displacements and magnetization and most importantly a coupling between the two is extremely rare. Previous theoretical proposals of cation-ordered \textit{SrCaRu}_2\textit{O}_6\textsuperscript{9} and \textit{BiPbTi}_2\textit{O}_6\textsuperscript{17} show the coexistence of ferromagnetism with polar displacements but there is no strong coupling between the two properties.

Recently, Princep and coworkers have synthesized a new polar metal \textit{Pb}_2\textit{CoOsO}_6 in which an antiferromagnetic order with magnetic frustration breaks the inversion symmetry\textsuperscript{19}. \textit{Pb}_2\textit{CoOsO}_6 crystallizes in a cation-ordered double-perovskite structure. At room temperature, the material is paramagnetic and centrosymmetric with space group \textit{P2}_1/\textit{n} (No. 14). At \(T = 45\) K, \textit{Pb}_2\textit{CoOsO}_6 undergoes a continuous phase transition to an antiferromagnetically ordered state with propagation vector \(\mathbf{k} = (1/2, 0, 1/2)\). Both \textit{Co} and \textit{Os} atoms have magnetic moments and they order simultaneously. Accompanying the appearance of magnetic order is the removal of inversion symmetry. This is because each \textit{Os} moment is surrounded by six neighboring \textit{Co} moments, three of which are parallel to the \textit{Os} moment and the other three of which are antiparallel to the \textit{Os} moment. The ferromagnetic and antiferromagnetic couplings between \textit{Os} and \textit{Co} moments are generically different and thus this magnetic frustration forces \textit{Os} moment to move away from the centrosymmetric position, which breaks the inversion symmetry. The low-temperature polar structure has space group \textit{Pc} (No. 7) with the corresponding Shubnikov group for the magnetic structure being \textit{Pac}. Since in \textit{Pb}_2\textit{CoOsO}_6 the polar displacements are induced by the unique long-range magnetic order, similar to “type-II multiferroics”\textsuperscript{20}, we may term \textit{Pb}_2\textit{CoOsO}_6 as
“type-II polar metals”, while SrCaRu$_2$O$_6$ and BiPbTi$_2$O$_6$ may be referred to as “type-I polar metals” since magnetic order and polar displacements have different sources and are weakly coupled in these materials.

In comparison with ferroelectrics, polar metals usually exhibit a much lower structural transition temperature, e.g. $T_s =$ 140 K for LiOsO$_3$ and $T_s (= T_N) =$ 45 K for Pb$_2$CoOsO$_6$ while the $T_s$ for a prototypical ferroelectric material BaTiO$_3$ is above room temperature. From the viewpoint of practical applications, it is desirable to increase the transition temperature of polar metals. By monitoring the resistivity anomaly at $T_s$ of LiOsO$_3$ under different pressures up to 6.5 GPa, Aulestia and coworkers has reported that the application of hydrostatic pressure can significantly enhance its non-polar to polar transition temperature with a linear slope of $dT_s/dP \approx 17.54$ K/GPa, reaching ca. 250 K at 6.5 GPa. Based on the first-principles calculations, the enhancement of $T_s$ in LiOsO$_3$ has been attributed to the fact that pressure stabilizes the polar metallic state with a smaller unit-cell volume than the non-polar state. The pressure effect of increasing $T_s$ in LiOsO$_3$ is different from that in BaTiO$_3$ in which pressure reduces its $T_s$.

In this work we study the pressure effect on the newly synthesized type-II polar metal Pb$_2$CoOsO$_6$ by monitoring the resistivity anomaly at $T_N$ under various pressures up to 11 GPa in a cubic anvil cell apparatus. We find that similar to LiOsO$_3$, the transition temperature $T_s = T_N$ is also increased by pressure. But interestingly, $T_N$ as a function of pressure $P$ increases with pressure with a discontinuous change of slope from $dT_N/dP = 6.8(8)$ K/GPa for $P < 4$ GPa to 1.8(4) K/GPa for $P > 4$ GPa. Our first-principles calculations suggest that the change of $dT_N/dP$ can be attributed to the vanishing of Os magnetic moment. Under pressure, Os moment is reduced and completely suppressed above a critical value. Above the critical pressure, the magnetic frustration is relieved and the inversion symmetry is restored, which leads to a distinct magnetic metallic state.

II. EXPERIMENTAL AND COMPUTATIONAL DETAILS

Pb$_2$CoOsO$_6$ single crystals were grown under high-pressure and high-temperature conditions as described elsewhere. Temperature dependences of magnetic susceptibility and resistivity at ambient pressure were measured on the Magnetic Properties Measurement System (MPMS-III) and Physical Property Measurement System (PPMS-9T) from Quan-
tum Design, respectively. We have carried out high-pressure resistivity measurements on Pb$_2$CoOsO$_6$ single crystals with standard four-probe method by using a palm cubic anvil cell (CAC) apparatus. Glycerol was employed as the pressure transmitting medium and the pressure values were determined from the pressure-loading force calibration curve at room temperature. Glycerol may produce some non-hydrostatic stress, but it is not expected to affect the reported results. Details about the experimental setup can be found elsewhere.

We perform spin polarized density functional theory (DFT) calculations using a plane wave basis set and projector-augmented wave method, as implemented in the Vienna Ab-initio Simulation Package (VASP). We take into account spin-orbit coupling (SOC) in the DFT calculations and test the Hubbard $U$ effect. We use PBEsol—a revised Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation for improving equilibrium properties of densely-packed solids as the exchange correlation functional. We start from the experimental crystal structure, and perform structural optimization under the studied pressures until each Hellmann-Feynman force component is smaller than $10^{-3}$ eVÅ$^{-1}$. We use the magnetic ordering obtained from experimental neutron powder diffraction in all our calculations, hence a very large cell with 80 atoms is used for the calculation. The Brillouin zone integration is performed with a Gaussian smearing of 0.05 eV over a Γ-centered $k$ mesh of $6 \times 12 \times 6$. An energy cutoff of 600 eV is used in all the calculations. The threshold of energy convergence is $10^{-7}$ eV. We use a higher energy cutoff (700 eV) and a denser $k$ mesh ($8 \times 14 \times 8$) and we do not find any significant changes in the key results. Our test calculations including Hubbard $U$ on Co and Os $d$ orbitals in the approach of Dudarev et al. find that electron correlation increases the magnetic moment on Co and Os. The DFT+$U$ calculations ($U_{Co} = U_{Os} = 2$ eV) find that the magnetic moments of Co and Os are 2.75 and 1.53 $\mu_B$, respectively. In particular, the magnetic moment of Os is about 3.6 times the DFT-calculated Os moment of 0.43 $\mu_B$, which strongly deviates from the experimental value (experimentally Os moment $< 0.5 \mu_B$). Hence all the computational results presented in this study are calculated by spin polarized DFT calculations without Hubbard $U$. 

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III. RESULTS AND DISCUSSION

The studied Pb$_2$CoOsO$_6$ single crystal was first characterized at ambient pressure by measuring the magnetic susceptibility $\chi(T)$ and resistivity $\rho(T)$. The results are consistent with those published in previous report\(^{19}\). As shown in Fig. 1, zero-field-cooled (ZFC) and field-cooled (FC) $\chi(T)$ curves measured under $\mu_0 H = 0.1$ T are almost overlapped with each other and both exhibit a clear cusp anomaly at the long-range antiferromagnetic transition at $T_N = 43$ K is marked by a vertical broken line.

FIG. 1: Temperature dependences of (a) magnetic susceptibility $\chi(T)$ and its inverse $\chi^{-1}(T)$, and (b) resistivity $\rho(T)$ and its derivative $d\rho/dT$ for the Pb$_2$CoOsO$_6$ single crystal. The antiferromagnetic transition at $T_N = 43$ K is marked by a vertical broken line.
order at $T_N = 43$ K. A Curie-Weiss fitting to $\chi^{-1}(T)$ in the paramagnetic region above 150 K yields an effective magnetic moment of $\mu_{\text{eff}} = 5.48 \, \mu_B$ per formula unit and a Curie-Weiss temperature of $\theta_{\text{CW}} = -89.2$ K, respectively. The obtained $\mu_{\text{eff}}$ is larger than the expected spin-only value of 4.8 $\mu_B$ by assuming high-spin Co(II) with $S = 3/2$ and Os(VI) with $S = 1$. This should be attributed to the fact that high-spin Co(II) in related double perovskites always have an effective moment higher than the spin-only value of 3.87 $\mu_B$ due to the presence of unquenched orbital moment. The negative $\theta_{\text{CW}}$ signals the presence of dominant net antiferromagnetic interactions that produce a moderate magnetic frustration, i.e. $|\theta_{\text{CW}}/T_N| \approx 2$ in this double perovskite. Pb$_2$CoOsO$_6$ is confirmed to be metallic in the whole temperature range and its $\rho(T)$ displays a clear inflection point at $T_N$, which can be defined clearly from the minimum of $\mathrm{d}^2 \rho / \mathrm{d}T^2$ as shown in Fig. 1(b). According to Ref.\textsuperscript{19}, the antiferromagnetic ordering involving both Co and Os sublattices will remove the inversion symmetry due to magnetic frustration, and relax the structure into a polar structure ($P_c$). Therefore, we can track the pressure dependence of the coupled antiferromagnetic/structural transition by monitoring the resistivity anomaly at $T_N$ under high pressures.

Figure 2(a) displays the $\rho(T)$ curves of Pb$_2$CoOsO$_6$ under various pressures up to 11 GPa. As can be seen, it remains metallic and the $\rho(T)$ decreases gradually with increasing pressure, in line with the general expectation that pressure broadens the electronic bandwidth. The resistivity anomaly at $T_N$ is clearly visible in the investigated pressure range and moves to higher temperatures with increasing pressure. This can be seen more clearly from the minimum of $\mathrm{d}^2 \rho / \mathrm{d}T^2$ curves in Fig. 2(b). The determined $T_N$ are plotted in Fig. 3(a) as a function of pressure. The transition temperature is almost doubled and reaches $\sim 80$ K at 11 GPa. Interestingly, it is found that $T_N(P)$ exhibits distinct pressure coefficients, i.e. $T_N(P)$ first increases with pressure in a large slope of +6.8(8) K/GPa for $P < 4$ GPa, and then in a much reduced slope of +1.8(4) K/GPa for $P > 4$ GPa.

In addition to the discontinuous slope change of $T_N(P)$, a closer inspection of the temperature dependence of $\rho(T)$ curves at low temperatures also evidenced a slope change for $P > 3$ GPa. To quantify this change, we have plotted the low-temperature $\rho(T)$ data in the form of $(\rho - \rho_0)$ versus $T^2$ in Fig. 2(c), which confirms that the Fermi-liquid behavior remains valid in the whole pressure range. The quadratic-temperature coefficient, $A$, determined from the linear fitting in Fig. 2(c) are shown in Fig. 3(b) as a function of pressure. A nonmonotonic evolution with pressure can be clearly seen at $\sim 4$ GPa. Similarly, $A(P)$ also
FIG. 2: Temperature dependences of (a) resistivity $\rho(T)$ and (b) its second derivative $d^2\rho/dT^2$ under various pressures up to 11 GPa for the Pb$_2$CoOsO$_6$ single crystal. (c) A plot of $\delta \rho \equiv (\rho - \rho_0)$ versus $T^2$ for the $\rho(T)$ data at low temperatures. The solid lines are linear fitting curves to extract the quadratic-$T$ coefficient $A$.

exhibits a discontinuous jump at $\sim 4$ GPa with distinct pressure coefficients, i.e. $dA/dP$ changes from $-6.7 \pm 1.8 \times 10^{-9}$ $\Omega$ cm K$^{-2}$ GPa$^{-1}$ at $P < 4$ GPa to $-2.2 \pm 0.7 \times 10^{-9}$ $\Omega$ cm K$^{-2}$ GPa$^{-1}$ at $P > 4$ GPa. Since the $A$ coefficient is proportional to the effective mass of charge carriers, the distinct values of $dA/dP$ imply that the impact of pressure on the electronic structure is altered significantly at $\sim 4$ GPa.

From these above measurements, we can reach the conclusion that the antiferromagnetic metallic state of Pb$_2$CoOsO$_6$ is stabilized by pressure, and it seems to enter a distinct state above 4 GPa as illustrated by the different pressure coefficients of $T_N(P)$ and $A(P)$. Since the polar state blow $T_N$ at ambient pressure is driven by the antiferromagnetic ordering involving both Co and Os sublattices, it is essential to understand how the magnetic state evolves under pressure in Pb$_2$CoOsO$_6$ in order to gain some insights on the overall structural properties, in particular polar distortions. However, direct measurements of long-range magnetic order
FIG. 3: Pressure dependence of (a) the antiferromagnetic transition temperature $T_N$ and (b) the quadratic-$T$ coefficient $A$ of Pb$_2$CoOsO$_6$ single crystal.

and magnetic moment (especially Os moment) is difficult, even under ambient conditions. Therefore we perform first-principles calculations in order to elucidate why a new distinct antiferromagnetic metallic state may emerge in Pb$_2$CoOsO$_6$ under pressure and to provide detailed electronic/magnetic/structural properties of pressurized Pb$_2$CoOsO$_6$, which are not easily measured in experiment.

First, we calculate the electronic structure of Pb$_2$CoOsO$_6$ under pressure. The optimized crystal structure of Pb$_2$CoOsO$_6$ at 0 K can be found in Table I in the Appendix. Figure
FIG. 4: The total density of states (DOS) of Pb$_2$CoOsO$_6$ under 0, 1, 3, 5, 7 and 9 GPa, obtained from (a) spin polarized DFT calculations and (b) DFT+SOC calculations. Note that in panel (a), the spin-up and spin-down are identical due to the antiferromagnetic ordering, thus they are summed in the DOS. The dashed line is the Fermi level.

4 shows the total density of states (DOS) of Pb$_2$CoOsO$_6$ under 0, 1, 3, 5, 7, and 9 GPa from DFT (Fig. 4(a)) and DFT+SOC (Fig. 4(b)) calculations. Because Pb$_2$CoOsO$_6$ has an antiferromagnetic ordering, the spin-up and spin-down are identical in spin polarized DFT calculations, hence the two spin-resolved DOS are summed in Fig. 4(a). In DFT+SOC calculations, $S_z$ is no longer a good quantum number and we show the total density of states (DOS). We find from both DFT and DFT+SOC calculations that the effect of pressure on the total DOS is very weak, similar to the previous study on LiOsO$_3$\cite{13}. Pb$_2$CoOsO$_6$ remains metallic under all the pressures in our study, consistent with the electrical transport
The lines are used to guide the eye.

measurements. While standard DFT calculations tend to underestimate band gaps, we also find robust metallic properties of Pb$_2$CoOsO$_6$ under pressure in our DFT+$U$ ($U_{Co} = U_{Os} = 2$ eV) calculations. By comparing the panels (a) and (b) of Fig. 4, we find that at a given pressure, the SOC effect on the total DOS is also very weak, especially its effect on the states close to the Fermi level.

Next, we consider the experimentally observed antiferromagnetic ordering in Pb$_2$CoOsO$_6$. Figure 5 shows the evolution of calculated magnetic moments of Co and Os under 0~9 GPa. DFT calculations and DFT+SOC calculations both predict that the magnetic moments of Co and Os decrease monotonically with increasing pressure. The SOC effect tends to decrease Os magnetic moment but increase Co magnetic moments. We find that from both DFT and DFT+SOC calculations, there exists a critical pressure $P_c$ ~ 8 GPa, above which Os magnetic moment vanishes, while Co moment only decreases slightly. This has important consequences on the magnetic transition temperature $T_N$. When the pressure is below the critical pressure, the Néel temperature $T_N$ of Pb$_2$CoOsO$_6$ is determined by the two-coupled magnetic sublattices ($i.e.$, Co and Os). However, above the critical pressure, $T_N$
FIG. 6: (a) The optimized crystal structure of Pb$_2$CoOsO$_6$ in an 80-atom cell and a metal-oxygen BO$_6$ octahedron ($B = \text{Co or Os}$). The polar displacement for the $B$-site metal ion is defined as: $\delta = \frac{1}{4} \sum_{i=1}^{4} d_i$, where $d_i = z_B - z_{O_i}$ and the index $i$ runs over 1 to 4 because there are four in-plane oxygen atoms in a BO$_6$ octahedron. In panel (a), only $d_1$ and $d_2$ are shown for clarity using the black double-headed arrows. (b) The average Co-O and Os-O polar displacements $\delta$ in Pb$_2$CoOsO$_6$ under 0∼9 GPa. The lines in the panel (b) are used to guide the eye.

is solely determined by the magnetic sublattice of Co. This may explain the discontinuity of $dT_N/dP$ under pressure in our experiments. We note that the critical pressure estimated from our calculations is larger than the critical pressure observed in experiment. This may result from the approximation of exchange-correlation functional in our first-principles calculations. While PBEsol improves the prediction of structural properties of solids, it may overestimate the intrinsic exchange splitting and possibly the magnitude of Os moment.

Finally, we study the structural properties of Pb$_2$CoOsO$_6$ under pressure. Because each Os moment is surrounded by six Co moments and these six Co moments form an antiferromagnetic ordering, a finite Os moment causes magnetic frustration in this double perovskite oxide and leads to polar distortions on both Os and Co atoms. We calculate the polar displacements of transition metal cations (Co and Os) $\delta$ along the $z$ direction. $\delta$ is defined as $\delta = \frac{1}{4} \sum_{i=1}^{4} d_i$, where $d_i = z_B - z_{O_i}$ and the index $i$ runs over 1 to 4 because there are four in-plane oxygen atoms in a CoO$_6$ or OsO$_6$ octahedron (see Fig. 6(a)). The polar displacement $\delta$ almost linearly decreases with the applied pressure up to 7 GPa, as is shown in Fig. 6(b). In the range of 0 ∼ 7 GPa, the Co polar displacements are substantially stronger (∼ 10 times) than the Os polar displacements. Our calculations further show that the Co-O and Os-O displacements simultaneously vanish at 8 GPa, coincident with the complete
suppression of Os moment. This is consistent with the picture that the inversion symmetry of Pb$_2$CoOsO$_6$ is broken by the magnetic frustration in the antiferromagnetic ordering\textsuperscript{[15].} With the Os moment vanishing, the magnetic frustration is relieved and thus the inversion symmetry is restored. In short, pressure drives Pb$_2$CoOsO$_6$ from an antiferromagnetic polar metal (with two types of magnetic ions) to an antiferromagnetic centrosymmetric metal (with only one type of magnetic ion).

IV. CONCLUSION

We perform transport and magnetic measurements and first-principles calculations to study the pressure effect on the recently synthesized type-II polar metal Pb$_2$CoOsO$_6$. Experimentally, we monitor the resistivity anomaly at the antiferromagnetic transition $T_N$ under various pressures up to 11 GPa, and found a discontinuous enhancement of $T_N(P)$ from 43 K at ambient pressure to $\sim$ 80 K at 11 GPa. The pressure coefficient of $T_N(P)$ decreases significantly from $dT_N/dP = 6.8(8)$ K/GPa for $P < 4$ GPa to $1.8(4)$ K/GPa for $P > 4$ GPa. Our first-principles calculations suggest that the observed discontinuity of $dT_N/dP$ around $\sim$ 4 GPa may be attributed to the disappearance of Os magnetic moment. Pressure substantially reduces the Os moment and above a critical value completely suppresses the Os moment. This relieves the magnetic frustration in the antiferromagnetic ordering of Pb$_2$CoOsO$_6$, which in turn decreases the Co-O and Os-O polar displacements. Above the critical pressure, both Co and Os atoms move to the centrosymmetric positions (i.e. the center of CoO$_6$ and OsO$_6$ octahedra) and the inversion symmetry is restored. This leads to a new antiferromagnetic metallic state in pressurized Pb$_2$CoOsO$_6$, distinct from the one under ambient pressure.

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Appendix A: The DFT optimized crystal structure of Pb$_2$CoOsO$_6$ and the discussion of Jahn-Teller distortions

Table I shows the optimized crystal structure obtained from our DFT calculations under 0 GPa. The DFT-calculated crystal structures of Pb$_2$CoOsO$_6$ under pressures up to 9 GPa are available in Ref.\textsuperscript{[35]}

We note that the Jahn-Teller distortions may be associated with the phase transitions in transition metal oxides under pressures\textsuperscript{[36]}, hence we study the possible Jahn-Teller distortions in CoO$_6$ and OsO$_6$ octahedra for the optimized structures under pressures. We follow Ref.\textsuperscript{[37]} and define a Jahn-Teller distortion parameter $\delta$ for both CoO$_6$ and OsO$_6$ octahedra: $\delta = \frac{l-s}{2(l+s)}$ where $l$ and $s$ are the longer and shorter $M$-O ($M = Os$ or $Co$) bond lengths in the $MO_4$ plane. Using this method, we find that the Jahn-Teller distortion $\delta$ for both CoO$_6$ and OsO$_6$ octahedra are on the order of $10^{-5}$ under pressures up to 9 GPa. This indicates that Jahn-Teller distortions in Pb$_2$CoOsO$_6$ are very weak both under ambient conditions and under pressures. Therefore, we can conclude that the Jahn-Teller distortion are not correlated to the observed magnetic transitions.

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TABLE I: The cell parameters of non-centrosymmetric Pb$_2$CoOsO$_6$: $a = 5.6984$ Å, $b = 5.6083$ Å, $c = 9.45938$ Å, $\alpha = \gamma = 90.0^\circ$, $\beta = 126.535^\circ$. The number of the space group of Pb$_2$CoOsO$_6$ is 7. Note that we use the setting of standard space group $P_c$ instead of the non-standard space group $P_n$ used in Ref.[19].

| Site | Wyckoff Positions | x      | y      | z      |
|------|-------------------|--------|--------|--------|
| Pb1  | 2a                | 0.26389| 0.25222| 0.25229|
| Pb2  | 2a                | 0.73935| 0.24779| 0.75099|
| Co   | 2a                | 0.00529| 0.75035| 0.00388|
| Os   | 2a                | 0.49961| 0.74996| 0.50011|
| O1   | 2a                | 0.19200| 0.74949| 0.25227|
| O2   | 2a                | 0.80921| 0.75062| 0.74717|
| O3   | 2a                | 0.29405| 0.00817| 0.03748|
| O4   | 2a                | 0.70126| 0.49262|-0.04084|
| O5   | 2a                | 0.29952| 0.49763| 0.03726|
| O6   | 2a                | 0.69581| 0.00158|-0.04061|

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