Electronic and magnetic properties of low-dimensional system Co$_2$TeO$_3$Cl$_2$

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Abstract

The electronic and magnetic properties of transition metal oxyhalide compound Co$_2$TeO$_3$Cl$_2$ are investigated using first principle calculations within the framework of density functional theory. To find the underlying spin-lattice of this compound, various hopping integrals and exchange interactions are calculated. The calculations reveal that the dominant inter-chain and intra-chain interactions are in the $ab$ plane. The exchange path is visualized by Wannier function plotting. The nearest neighbor and next nearest neighbor exchange interactions are antiferromagnetic, making the system frustrated in low dimension. Calculations are also done with spin–orbital coupling (SOC) to find out the effect of SOC on this compound. Calculation of magnetocrystalline anisotropy suggests that the easy axis is along the crystallographic $b$ direction.

Keywords: magnetism, antiferromagnetism, low dimensional spin system, exchange interaction, spin–orbit coupling, density functional theory

(Some figures may appear in colour only in the online journal)

1. Introduction

Low-dimensional spin systems have attracted much attention over the past few decades due to their variety of unusual magnetic properties [1–5]. Effective low dimensionality means anisotropic exchange interactions in different directions of the crystal that arises due to the interplay of geometry and chemical bonding. A system is known as low dimensional if the dominant exchange interactions are along intra-chain (1D) or intra-plane (2D) [1, 6]. Due to enhanced quantum fluctuations in low dimension, exotic properties can be seen in these class of materials. The presence of magnetic frustration in low-dimensional spin systems is particularly important. Many complex compounds with different spin lattices like spin ladder, Kagome lattice, triangular lattice, spin chain show fascinating magnetic properties like spin gap state, spin liquid state, various type of complex magnetic order etc [7–11]. Transition metal oxyhalide compounds comprising a p-element having a stereochemically active lone pair (such as Te$^{4+}$, Se$^{4+}$, Sb$^{3+}$ etc) form an attractive field of study. There is a high probability of finding new low-dimensional and frustrated spin system in these class of materials. The example of such systems are: FeTe$_2$O$_5$Br, Cu$_2$Te$_2$O$_5$Cl$_2$, Ni$_5$(TeO$_3$)$_4$Cl$_2$, etc [12–14]. Due to reduced dimensionality and geometric frustration, these materials often show complex magnetic order and interesting magnetic properties. Some of these materials also show multi-ferroic property [15, 16]. Number of such oxyhalide compounds are synthesized and studied over time. However, the family of Co$^{2+}$ containing oxohalogenides including a lone-pair cation is not studied much. Co$_2$TeO$_3$Cl$_2$ is one such compound which is synthesized by Becker et al [17]. It has a layered structure. The magnetic properties measurements by them suggest long range antiferromagnetic interactions below 30 K and the Curie–Weiss temperature is $-97$ K [17]. Neutron diffraction study of a powder sample suggests that Co spins are parallel to the crystallographic $b$ directions [18]. The exact spin-lattice of the system is not known. In complex crystal structures, the microscopic understanding of the spin-lattice remains a challenging problem. The knowledge of intra-chain and inter-chain exchange interactions is crucial to understand the magnetic behavior of these materials. *Ab initio* calculations play important role in this direction.
In this paper, the electronic and magnetic properties of Co$_2$TeO$_3$Cl$_2$ are studied using first principle calculations within the framework of density functional theory (DFT). To determine the underlying spin-lattice of this compound, various hopping integrals and exchange interactions between Co$^{2+}$ ions are calculated. In order to study the importance of spin–orbit coupling (SOC) in this system, the electronic structure calculations are also carried out with SOC, and magnetic anisotropy energy is calculated. The remainder of the paper is organized as follows: the crystal structure and method are discussed in section 2. The results of electronic structure calculations are discussed in section 3. Finally, the results are summarized in section 4.

2. Crystal structure and method

Co$_2$TeO$_3$Cl$_2$ (see figure 1) crystallizes in the monoclinic structure with space group P2$_1$/m (No. 11). The lattice parameters are $a = 5.0472$ Å, $b = 6.6325$ Å, $c = 8.3452$ Å, and $\beta = 105.43^\circ$ [17]. There are two crystallographically different Co ions in this system. Co1 is in square planar environment with two oxygen ions (O1) at a distance of 2.053 Å and other two oxygen ions (O2) at a distance of 2.084 Å. Further Co1 is coordinated by two chlorine atoms at a distance of 2.497 Å, forming Co1O$_2$Cl$_2$ octahedron. The Co2 atom is coordinated by three oxygen atoms (two O1 and one O2) and to three chlorine atoms and forming Co2O$_2$Cl$_3$ octahedron. The Co1O$_2$Cl$_2$ octahedra share edges with Co2O$_2$Cl$_3$ octahedra and form a layered structure. These layers are connected by Te ions. In a layer, the nearest Co1–Co2 distance is 3.06 Å. Figure 1(b) shows the arrangement of Co ions in a layer.

In the present study, electronic structure calculations are carried out using two different basis sets: (i) the muffin-tin orbital based linearized muffin-tin orbital (LMTO) method within atomic sphere approximation (ASA) and Nth order muffin-tin orbital (NMTO) downfolding method as implemented in the Stuttgart code [19–21] and (ii) the plane wave based projector augmented wave (PAW) [22] method as implemented in the vasp code [23]. The appropriate empty spheres are inserted in the interstitial regions to get the space filling in LMTO-ASA calculations. The basis set for the self-consistent electronic structure calculation for Co$_2$TeO$_3$Cl$_2$ in the LMTO method includes Co ($s$, $p$, $d$), Te ($s$, $p$, $d$), Cl ($s$, $p$), and O ($s$, $p$) and the other orbitals are downfolded. The self-consistency is achieved by Brillouin-zone integrations in a $(8 \times 8 \times 8)$ $k$ point mesh. The NMTO downfolding method [21], where potentials are taken from self-consistent LMTO method, is used to derive the low energy Hamiltonian. In this method, the low energy model Hamiltonian is constructed by selective downfolding method, where high energy degrees of freedom are integrated out from the all orbital local density approximation (LDA) calculations.

For the calculations using plane wave based method, the wave functions are expanded in the plane-wave basis with a kinetic energy cutoff of 500 eV. The exchange-correlation functional is chosen to be the Perdew–Burke–Ernzerhof implementation of the generalized gradient approximation (GGA) [24]. To properly describe the electron correlation associated with the 3$d$ states of Co, GGA + U method is used in the calculations [25]. For electronic structure calculations with SOC, it is included in scalar relativistic form as a perturbation to the original Hamiltonian. The structural relaxations are carried out until the Hellman–Feynman forces became less than 0.01 eV Å$^{-1}$. The calculation revealed that there is very small deviation of the atomic position in the relaxed structure from experimental structure. Therefore experimental lattice parameters and atomic positions are used for all the calculations.

3. Results and discussion

3.1 Spin-unpolarized calculation

To begin with, the electronic structure of Co$_2$TeO$_3$Cl$_2$ is studied without magnetic order. The total and orbital projected density of states (DOS) are displayed in figure 2(a). Non-magnetic DOS reveals that the Fermi level ($E_F$) is dominated by partially filled Co–$d$ orbitals. Since the oxidation states of O and Cl ions are −2 and −1 respectively, the O–$p$ and Cl–$p$ states are fully occupied. The O–$p$ states overlap
with Co-$d$ states indicating the strong hybridization of Co-$d$ states with O-$p$ states. As expected, the occupied Te-$s$ states lie far below the Fermi level and empty Te-$p$ states lie above $E_F$, spreading in the energy range of 2–5 eV. The Te-5$s$ and Te-5$p$ states are strongly hybridized with the O-$p$ states, which in turn hybridize with Co-$d$ states near the Fermi level. The system is metallic for the spin unpolarized calculation within LDA. The spin unpolarized bandstructure calculated within LMTO method is displayed in figure 2(b). The bands are plotted at the various high symmetry points of the Brillouin zone corresponding to the monoclinic lattice. The Fermi level is dominated by Co-$d$ states hybridized with O-$p$ and Cl-$p$ states.

### 3.2. Crystal field splitting and magnetism

The NMTO downfolding calculations are performed in order to find the crystal field splitting of Co-$d$ orbitals and hopping interactions between Co ions. To calculate crystal field splitting, only Co-$5d$ orbitals are retained in the basis and the rest are downfolded. The diagonalization of the onsite block of $5 \times 5$ Hamiltonian gives the crystal field splitting for Co1-$d$ and Co2-$d$ states including the covalency with oxygens and chlorines. These energies are calculated to be ($-2.76, -2.69, -2.58, -1.72$ and $-1.41$ eV) and ($-2.63, -2.61, -2.28, -1.83$ and $-1.43$ eV) for Co1 and Co2 respectively. The corresponding eigenstates turn out to be of mixed character and nondegenerate. The eigen states of Co1 and Co2 are following:

\[
\begin{align*}
(1') &= -0.93|xy\rangle + 0.34|yz\rangle \\
(2') &= 0.30|z^2 - r^2\rangle - 0.92|xz\rangle - 0.34|x^2 - y^2\rangle \\
(3') &= -0.34|xy\rangle - 0.93|yz\rangle \\
(4') &= -0.38|z^2 - r^2\rangle - 0.68|xz\rangle + 0.61|x^2 - y^2\rangle \\
(5') &= 0.66|z^2 - r^2\rangle + 0.02|xz\rangle + 0.74|x^2 - y^2\rangle
\end{align*}
\]

The level diagram of crystal field splitting and the filling of electrons (including spin polarization) in the $d$ level of Co1 and Co2 are shown in figure 3. There are three partially filled $d$-orbitals in the Co ions, that are retained in the low energy model and the other orbitals are downfolded. The downfolded bandstructure calculated with all orbital bandstructure is displayed in figure 4. The Fourier transformation of the low energy model Hamiltonian, \( H_R = \sum_{ij} t_{ij} (c_i^\dagger c_j + H.C.) \) gives the hopping integrals between various Co atoms. The hopping integrals are displayed in table 1. The next nearest neighbor (nnn) hopping interaction ($t_2$) turns out to be strongest. The nearest neighbor (nn) interaction $t_1$, between Co1 and Co2, is compared to the nnn hopping interaction. The strongest hopping $t_2$ is between two corner sharing Co1 octahedra and this hopping is primarily mediated by O2 situated on the basal
plane of the Co1 octahedron, forming a strong \( p_d \sigma \) antibond with the Co-\( d \) orbital. Whereas, the nearest neighbor hopping \( t_1 \) is between the edge sharing Co1 and Co2 octahedra. The hopping strength, as well as the strength of exchange interactions, strongly depend on the bond angle and bond distances. The bond angle of Co1–O2–Co1 corresponding to \( t_2 \) hopping is 105.5°, while the bond angles for \( t_1 \) hopping path are \( \angle \text{Co1–O1–Co2} = 95.5° \) and \( \angle \text{Co1–O5–Co2} = 81.93° \). When the bond angle is close to 90°, due to the orthogonality of Co-3\( d \) and O-2\( p \) orbitals, antiferromagnetic super-exchange interaction reduces. Therefore the antiferromagnetic part of exchange coupling along the path \( t_1 \) is expected to be smaller than the antiferromagnetic part of exchange coupling along the path \( t_2 \). Other hoppings, \( t_3 \) and \( t_4 \) are smaller compared to \( t_1 \) and \( t_2 \) but non-negligible. Other hoppings in \( ab \) plane are

Table 1. Calculated hopping integrals (in meV) for Co\(_2\)TeO\(_3\)Cl\(_2\) are listed here. The interaction paths (\( t_1, t_2 \) and \( t_3, t_4 \)) are indicated in figure 1(b).

| Hopping Ing. | Atoms       | Distance (Å) | Orbital involved |
|--------------|-------------|--------------|------------------|
| \( t_1 \)    | Co1–Co2    | 3.01         | \( |1\rangle \) \( |2\rangle \) \( |3\rangle \) \( |1\prime\rangle \) \( |2\prime\rangle \) \( |3\prime\rangle \) |
|              |             |              | \( -22.6 \) \( 0 \) \( -63.3 \) \( 28 \) \( 15.4 \) \( 30 \) \( -38.4 \) \( -80.2 \) \( -5.1 \) |
| \( t_2 \)    | Co1–Co1    | 3.31         | \( |1\rangle \) \( |2\rangle \) \( |3\rangle \) \( |1\prime\rangle \) \( |2\prime\rangle \) \( |3\prime\rangle \) |
|              |             |              | \( 47.8 \) \( 23.1 \) \( 23 \) \( -23.1 \) \( -42.8 \) \( -42.9 \) \( -23 \) \( -42.9 \) \( -83.8 \) |
| \( t_3 \)    | Co1–Co2    | 4.12         | \( |1\rangle \) \( |2\rangle \) \( |3\rangle \) \( |1\prime\rangle \) \( |2\prime\rangle \) \( |3\prime\rangle \) |
|              |             |              | \( -19.3 \) \( -29.3 \) \( 21.1 \) \( -31.7 \) \( -58.5 \) \( 54.2 \) \( -11.3 \) \( 43.3 \) \( 25 \) |
| \( t_4 \)    | Co2–Co2    | 5.05         | \( |1\prime\rangle \) \( |2\prime\rangle \) \( |3\prime\rangle \) \( |1\prime\rangle \) \( |2\prime\rangle \) \( |3\prime\rangle \) |
|              |             |              | \( -19.3 \) \( -31.7 \) \( -11.3 \) \( -29.3 \) \( -58.5 \) \( 43.3 \) \( 21.1 \) \( 54.2 \) \( 25 \) |

Figure 4. The downfolded bandstructure (red line) compared with full LDA bandstructure (black line) of Co\(_2\)TeO\(_3\)Cl\(_2\).

Figure 5. Plot of Wannier functions placed at two different Co sites. The two oppositely signed lobes of the wave functions at site 1 (2), are colored differently as black (magenta) and grey (cyan). (a) Overlap of Co1-\( xy \) orbital with Co2-\( x^2−y^2 \) and (b) overlap of Co1-\( xy \) orbital with Co2-\( 3z^2−1 \).

Figure 6. The spin polarized density of states for Co\(_2\)TeO\(_3\)Cl\(_2\). (a) Total DOS. Orbital projected DOS for (b) Co-\( d \), (c) Te-\( s \) and Te-\( p \), (d) O-\( p \) and Cl-\( p \) states.
negligible. The hopping along crystallographic c direction is also negligible. The strength of the intra-chain and inter-chain hoppings indicate that this system is low dimensional. The antiferromagnetic part of the exchange interactions can be calculated from the hopping integrals using the expression [26]:

\[ J_{AF} = \sum_{ij} t_{ij}^2 U + \Delta_{nn} \]

where, \( U \) is the Coulomb interaction and \( \Delta_{nn} \) is the onsite energy difference. \( U = 4 \text{ eV} \) and \( \Delta_{nn} = 0.3 \text{ eV} \) are taken in the calculation. The antiferromagnetic part of the exchange interactions are tabulated in the last column of table 3.

In order to visualise the dominant interactions paths, the Wannier functions corresponding to the nearest neighbour Co1 and Co2 ions are plotted in figure 5. Figure 5(a) reveals that the overlap between Co1-\( d_{xy} \) effective Wannier functions and that between Co2-\( d_{x^2-y^2} \) Wannier functions, placed at two nearest-neighbor Co sites within the chain. These two Co atoms are connected by three oxygens. The super exchange path of \( t_1 \) hopping is Co1–O–Co2. Additionally they are connected also by Cl atom. Each Co \( d \) orbitals form strong \( pd\sigma \) antibonding linkages with the neighboring \( Op_e/p_{ty} \) orbitals. The tails of the two Co Wannier functions overlap at the Cl site connecting two Co atoms, forming the crucial exchange path. Wannier function of Co2-\( d_{3z^2-r^2} \) is plotted in figure 5(b).

### Table 3. The exchange interactions (meV) are listed here.

| Exchange path | Distance (Å) | Type of Co atom | Total exchange | \( J_{AF} \) from NMTO |
|--------------|--------------|----------------|----------------|------------------------|
| J1          | 3.01         | Co1–Co2 intra-chain | −6.01          | −7.3                   |
| J2          | 3.31         | Co1–Co1 intra-chain | −7.12          | −8.7                   |
| J3          | 4.12         | Co1–Co2 intra-chain | 3.83           | −2.4                   |
| J4          | 5.05         | Co2–Co2 inter-chain | −4.76          | −3.7                   |

### Table 4. The spin (orbital) moment of Co\(^{2+}\) ions, energy difference (in meV) within GGA + U + SOC calculations (with \( U_{\text{eff}} = 4 \text{ eV} \) ion axis are listed here.

| Spin quantization axis | Co1 moment (\( \mu_B \)) | Co2 moment (\( \mu_B \)) | \( \Delta E \) |
|------------------------|--------------------------|--------------------------|--------------|
| (0 0 1)                | 2.7 (0.21)               | 2.7 (0.22)               | 0            |
| (0 1 0)                | 2.66 (0.22)              | 2.67 (0.22)              | −2.20        |
| (1 0 0)                | 2.66 (0.22)              | 2.65 (0.22)              | −1.20        |

### 3.3. Spin polarized calculations

Next, the electronic structure of Co\(_2\)TeO\(_3\)Cl\(_2\) has been investigated with magnetic order. Figure 6 displayed the spin polarized total and orbital decomposed density of states calculated within GGA + U. For these calculations, the on-site Coulomb interaction (\( U \)) for Co is taken to be \( U = 5 \text{ eV} \) and the on-site exchange interaction \( J_H = 1 \text{ eV} \) i.e. \( U_{\text{eff}} = 4 \text{ eV} \) [27, 28]. DOS reveals that the majority spin of Co-\( d \) states are completely...
occupied and minority spin states are partially occupied and this picture is consistent with high spin state of Co$^{2+}$ ion. The magnetic moment of states are spread over the energy range $-6$ to $6$ eV.

As discussed above that the angles involved in the exchange paths much deviate from $90^\circ$ (or $180^\circ$), Goodenough–Kanamori–Anderson (GKA) rule [29, 30] can not be applied here. The nature of the interaction between $d^2$–$d^7$ orbital mainly governed by the exchange path and angle with the bridging oxygen atom. In order to find out total magnetic exchange interactions between Co$^{2+}$ ions, total energy calculation method is adopted here [5, 10, 11, 31, 32]. In this method, the total energies are calculated for several ordered spin configurations of a system and then related the energy differences between these configurations to the corresponding energy differences expected from the Heisenberg spin Hamiltonian: \[
H = -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j.
\]
The plane wave basis set is used for this calculations. From the hopping strengths, one can conclude that there are four dominant exchange interactions for this system as indicated in figure 1. Five different magnetic configurations (see figure 7) are made to find out four dominant exchange interactions. $2 \times 1 \times 1$ supercell is used to make different antiferromagnetic arrangements. In AF1 configuration, Co1 spins are antiferromagnetically coupled with Co2 spins, whereas in AF2 configuration, Co1 spins are antiparallel along the $a$ direction and all four Co2 spins are parallel with each other. In AF3 configuration, Co2 spins are antiparallel along $a$ and $c$ directions and Co1 spins are antiparallel only along the $b$ direction. AF4 configuration is similar to AF3 configuration except, Co1 spins are aligned antiferromagnetically along $a$ and $b$ directions in AF4 configuration. The energy difference of antiferromagnetic configurations with ferromagnetic configuration, bandgap, magnetic moments in each configuration are displayed in table 2. The total energies with N unpaired spins per spin site ($N=3$) of these configurations are written as:

\[
E(FM) = -(8J_1 + 4J_2 + 8J_3 + 8J_4) \frac{N^2}{4}
\]

\[
E(AF1) = -(-8J_1 + 4J_2 - 8J_3 + 8J_4) \frac{N^2}{4}
\]

\[
E(AF2) = -4J_2 \frac{N^2}{4}
\]

\[
E(AF3) = -(8J_1 + 4J_2 - 8J_3 - 8J_4) \frac{N^2}{4}
\]

\[
E(AF4) = -8J_4 \frac{N^2}{4}
\]

$J_1$, $J_2$, $J_3$ and $J_4$ are calculated from the above equations. The calculated exchange energies are listed in table 3.

The result of the calculations reveal that the nearest neighbour (nn) interaction $J_1$ between Co1 and Co2 is antiferromagnetic. Next nearest neighbour (nnn) interaction $J_2$ between Co1–Co2 is also antiferromagnetic and stronger than $J_1$ interaction. Due to corner sharing topology of two Co2 octahedra, antiferromagnetic type $J_2$ is stronger than $J_1$. The inter chain exchange interaction $J_3$ is between Co1–Co2 and it is ferromagnetic type. Another inter chain exchange interaction $J_4$ between Co2–Co2 is also antiferromagnetic and comparable to intra chain exchange interactions. Such strong antiferromagnetic interactions make the system frustrated in low dimension.

### 3.4. Spin–orbit coupling

Spin–orbit coupling plays an important role in Co and Co based compounds,[11, 28, 33–35] In order to investigate the effect of spin–orbit coupling on Co$_2$TeO$_3$Cl$_2$, the electronic structure calculations are carried out within GGA $+ U$ calculation. The Te-s states are completely occupied and lie far below the Fermi energy. The O-p and Cl-p states are spread over the energy range $-6$ to $6$ eV.

As discussed above that the angles involved in the exchange paths much deviate from $90^\circ$ (or $180^\circ$), Goodenough–Kanamori–Anderson (GKA) rule [29, 30] can not be applied here. The nature of the interaction between $d^2$–$d^7$ orbital mainly governed by the exchange path and angle with the bridging oxygen atom. In order to find out total magnetic exchange interactions between Co$^{2+}$ ions, total energy calculation method is adopted here [5, 10, 11, 31, 32]. In this method, the total energies are calculated for several ordered spin configurations of a system and then related the energy differences between these configurations to the corresponding energy differences expected from the Heisenberg spin Hamiltonian: \[
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The plane wave basis set is used for this calculations. From the hopping strengths, one can conclude that there are four dominant exchange interactions for this system as indicated in figure 1. Five different magnetic configurations (see figure 7) are made to find out four dominant exchange interactions. $2 \times 1 \times 1$ supercell is used to make different antiferromagnetic arrangements. In AF1 configuration, Co1 spins are antiferromagnetically coupled with Co2 spins, whereas in AF2 configuration, Co1 spins are antiparallel along the $a$ direction and all four Co2 spins are parallel with each other. In AF3 configuration, Co2 spins are antiparallel along $a$ and $c$ directions and Co1 spins are antiparallel only along the $b$ direction. AF4 configuration is similar to AF3 configuration except, Co1 spins are aligned antiferromagnetically along $a$ and $b$ directions in AF4 configuration. The energy difference of antiferromagnetic configurations with ferromagnetic configuration, bandgap, magnetic moments in each configuration are displayed in table 2. The total energies with N unpaired spins per spin site ($N=3$) of these configurations are written as:

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\]

\[
E(AF1) = -(-8J_1 + 4J_2 - 8J_3 + 8J_4) \frac{N^2}{4}
\]

\[
E(AF2) = -4J_2 \frac{N^2}{4}
\]

\[
E(AF3) = -(8J_1 + 4J_2 - 8J_3 - 8J_4) \frac{N^2}{4}
\]

\[
E(AF4) = -8J_4 \frac{N^2}{4}
\]

$J_1$, $J_2$, $J_3$ and $J_4$ are calculated from the above equations. The calculated exchange energies are listed in table 3.

The result of the calculations reveal that the nearest neighbour (nn) interaction $J_1$ between Co1 and Co2 is antiferromagnetic. Next nearest neighbour (nnn) interaction $J_2$ between Co1–Co2 is also antiferromagnetic and stronger than $J_1$ interaction. Due to corner sharing topology of two Co2 octahedra, antiferromagnetic type $J_2$ is stronger than $J_1$. The inter chain exchange interaction $J_3$ is between Co1–Co2 and it is ferromagnetic type. Another inter chain exchange interaction $J_4$ between Co2–Co2 is also antiferromagnetic and comparable to intra chain exchange interactions. Such strong antiferromagnetic interactions make the system frustrated in low dimension.

### 4. Summary and conclusion

First principles electronic structure calculations are carried out to study the electronic structure and magnetic properties of oxyhalide compound Co$_2$TeO$_3$Cl$_2$. In order to determine the underlying spin-lattice, various hopping integrals and exchange interactions between Co$^{2+}$ ions are calculated. Hopping integrals calculated using the NMTO downfolding method reveal that both intra-chain and inter-chain hoppings in the $ab$ plane are comparable and therefore the system is low dimensional. The dominant exchange interactions are found to be antiferromagnetic. The nearest neighbor interaction $J_1$ and next nearest neighbor interaction $J_2$ are antiferromagnetic, making the system frustrated. $J_3$ is stronger than $J_1$. Results of the present work suggest that the system is two dimensional with competing magnetic interactions. The importance of spin–orbit coupling in this compound is also investigated. The results of calculations reveal that magnetocrystalline anisotropy is strong in Co$_2$TeO$_3$Cl$_2$ and (0 1 0) is the easy axis as observed experimentally.

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