Layered van der Waals topological metals of TaTMTe$_4$ (TM = Ir, Rh, Ru) family

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Layered van der Waals materials of the family TaTMTe$_4$ (TM=Ir, Rh, Ru) are showing very interesting electronic properties. Here we report the synthesis, crystal growth and structural characterization of TaIrTe$_4$, TaRhTe$_4$, Ta$_{1+x}$Rh$_{1-x}$Te$_4$ ($x = 0.06$; $0.14$; $0.78$; $0.92$) and Ta$_{1+x}$Ru$_{1-x}$Te$_4$ single crystals. X-ray powder diffraction confirms that TaRhTe$_4$ is isosstructural to TaIrTe$_4$. We show that all these compounds are metallic with diamagnetic behavior. Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ exhibits an upturn in the resistivity at low temperatures which is strongly field dependent. Below $T \approx 4K$ we observed signatures of the superconductivity in the TaIr$_{1-y}$Rh$_y$Te$_4$ compounds for $x = 0.92$. Magnetotransport measurements on all samples show weak magnetoresistance (MR) field dependence that is typically quadratic-in-field. However, for Ta$_{1-y}$Rh$_y$Te$_4$ with $x \approx 0.78$, the MR has a linear term dominating in low fields that indicates the presence of Dirac cones in the vicinity of the Fermi energy. For TaRhTe$_4$ series the MR is almost isotropic. We have performed electronic structure calculations for isosstructural TaIrTe$_4$ and TaRhTe$_4$ together with the projected total density of states. The main difference is appearance of the Rh-band close to the Fermi level.

I. INTRODUCTION

Layered van der Waals two dimensional materials with sizable spin-orbit coupling effects such as WTe$_2$ and MoTe$_2$, have been showing a wide array of fascinating properties, which might be deliberately modified by a variety of parameters, such as composition, thickness, etc [1] makes them even more attractive to gain insight into those physical effects. Recent reports demonstrate type II Weyl semimetallic behavior, both theoretically and experimentally, in both T$_d$-MoTe$_2$ and WTe$_2$ compound [2–5]. MoTe$_2$ is also found to host an edge supercurrent [6], to be superconductive [7] with strong enhancement of $T_c$ in point-contact measurements [8] and with sulfur substitution [9] and in monolayers [10]. Moreover, MoTe$_2$ and WTe$_2$ exhibit reversible metal-insulator transition, making them attractive candidates for two-dimensional nanoelectronics [11, 12]. WTe$_2$ shows similar array of properties: the compound is known to host quantum spin Hall state [13], and has large non-saturating magnetoresistance (MR) [14, 15]. Another feature of this structure is the possibility of formation of polar domains. As reported in [16, 17], WTe$_2$ and MoTe$_2$ demonstrate switchable spontaneous polarization and a natural ferroelectric domain structure, WTe$_2$ even at room temperature. Combined with metallic conductivity, this makes those materials first reported real-world examples of a ferroelectric metal materials.

Due to all the fascinating properties the search for materials with similar crystal structure is an active area of research. TaIrTe$_4$ structure can be derived from WTe$_2$ by substituting all W atoms with Ta and Ir ordered into zigzag chains along a direction, where Ir and Ta atoms alternating along the chain (Fig. 1) [18, 19]. TaIrTe$_4$ has been predicted to host Weyl fermions [20], hosting only four Weyl points (WPs), the minimal number of WPs a WSM with time-reversal invariance can host. Later on signatures of the WPs were found in ARPES [21]. Thickness-related properties were also reported, e.g. in mono- and bilayer TaIrTe$_4$ quantum hall effect was reported [22], while bulk crystals show room-temperature nonlinear Hall effect with temperature-induced sign change [23]. Moreover TaIrTe$_4$ is reported to host surface superconductivity with critical temperatures of up to 1.54K [24]. Among other members of this ternary telluride family NbIrTe$_4$ was proposed to host type-II Weyl fermions with experimental indica-

![FIG. 1. Schematics of crystal structure of TMTe$_2$ and TaTMTe$_4$ compounds. M$^1$=M$^3$=W in case of WTe$_2$ and M$^1$=TM, M$^3$=Ta for TaTMTe$_4$. Note the reduced distance between M$^1$ and M$^2$ forming a zigzag chains along a.](image-url)
tions in charge transport measurements [25]. This material also demonstrates non-saturating MR [26]. Recently both binary (WTe₂, MoTe₂) and ternary (TaTMTe₄, TM=Ir, Rh, Ru) tellurides showed bi-stable resistive metal-insulator switching in point contact measurements at room temperature, bringing those materials closer to applications. [12]

Original reports of the TaIrTe₄ structure also asserts the existence of several other MMTe₄ compounds and authors furthermore show that among other compounds TaRhTe₄ and TaRuTe₄ exist and suggest that TaRhTe₄ might be isostuctural to TaIrTe₄, while TaRuTe₄ might be disordered analogue of the TaIrTe₄. [18, 19] This wide array of iso- or similarly structured compounds makes this family a large playground to study the dependence of physical properties on parameters such as lattice size, interatomic distances, outer shell electron number, etc. Beyond initial structural studies of powder samples no further characterization of structural and physical properties on single crystals have been reported. Further chemical and structural investigation of those compounds provides better description of the material at hand, as well as more precise input parameters for theory models.

Here we report crystal growth of 3 members of TaTMTe₄ family, i.e. TaIrTe₄, TaRhTe₄ and Ta₁₋ₓRuₓTe₄ and Ta₁₋ₓRuₓTe₄. Also, we have successfully grown single crystals of doped series such as Ta₁₋ₓRhₓTe₄. Further, we discuss composition of acquired samples which is followed by an assessment of the structure of the materials with x-ray and electron diffraction methods. Finally we report results of magnetotransport measurements for selected crystals.

II. EXPERIMENTAL

A. crystal growth

Single crystals of TaIrTe₄, TaRhTe₄, and Ta₁₋ₓRuₓTe₄ were grown via self-flux method. Powders of Ta (Alfa Aesar, powder 325 mesh, 99.97%), transition metal, TM–Ir (Alfa Aesar, powder 325 mesh, 99.9%), Rh (Evochem, powder, 99.95%), Ru (MaTecK, powder, < 60µm, 99.9%) correspondingly, and Te (Alfa Aesar, powder 18 mesh, 99.999%) were mixed in Ta:TM:Te=1:1:20 molar ratio and thoroughly ground by hand in agate mortar. Afterwards reaction mixture was loaded into Canfield crucible set [27], which in turn was placed in evacuated fused quartz ampule. The mixture was heated up to 970°C at 100°C/h, dwelled at this temperature for 24 h, and subsequently slowly cooled at the rate of 1.5°C/h to final temperature of 600°C. Further, the crucible was taken out of hot furnace, turned over and instantly put to a centrifuge which facilitated flux removal. Afterwards, crystal surfaces contaminated by small amount of the flux were mechanically cleaved off before further studies. Furthermore, a substitution series of Ta₁₋ₓRhₓTe₄ was synthesized. For growth of this substitution series mixture of elemental powders with molar ratio Ta₁₋ₓRhₓ−₁Te₄=x:Te=1:1:20 for x = 0.1, 0.3, 0.7 and 0.9 was prepared as described for ternary compounds, after which the mixture was heated to 1000°C, held at this temperature for 24 h, and then cooled over course of 133 h to 700°C, after which the reaction mixture was centrifuged in aforementioned manner.

B. characterization

1. composition and structure

The composition of the as grown single crystals was determined by energy-dispersive x-ray spectroscopy (EDX), employing an electron beam probe in a scanning electron microscope (accelerating voltage 30kV, current 552pA). Structural characterization and phase purity was confirmed by means of powder X-ray diffraction using a STOE powder diffractometer (Bragg-Brentano transmission geometry, 2θ:ω scan, Co Kα1 or Mo Kα1 radiation, curved Ge (111) monochromator). Rietveld refinement of the x-ray data was carried out with FullProf [28] and Jana2006 [29] software packages.

Selected area electron diffraction (SAED) on thin exfoliated TaTMTe₄ (TM=Ir, Ru, Rh) was utilized by employing FEI Tecnai F20 transmission electron microscope (TEM) with LaB₆ emitter operated at 200 kV acceleration voltage. The TaTMTe₄ crystals used in this work were mechanically exfoliated using commercially available adhesive tape (eco, tesa). The exfoliated TaTMTe₄ crystals were separated from the tape by immersion in 10 mL of acetone and isopropanol (1:1) solution in 12 mL glass sample vial. Ultrasonication (frequency ≈ 35 kHz) was employed to assist the separation of TaTMTe₄-flakes from the tape surface for two hours (8 × 15 minutes sonication process with 5 minutes breaks between the 15 minutes session). The micrometer-sized TaTMTe₄ flakes were then transferred to the TEM lacey-carbon Cu grids using a standard pipette. To ensure the cleanliness of the TaTMTe₄-flakes the elemental composition of every TaTMTe₄-flake was confirmed by in-situ TEM-EDX before collection of the SAED pattern. Theoretical kinematic electron diffraction patterns were computed and visualized using the SingleCrystal software package version 3.1.5, (CrystalMaker Software Ltd., UK).

2. physical properties

Magnetic susceptibility was measured using a MPMS superconducting quantum interference device (SQUID) magnetometer from Quantum Design. Transport and magnetotransport measurements with TaTMTe₄ compounds were performed in fields up to 9 T using a PPMS-9 system from Quantum Design, and up to 16 T using...
CFMS-16 system from Cryogenic respectively. Temperature dependencies of the longitudinal resistivity $\rho_{xx}$ were measured in the temperature range 2–300 K, and angular dependencies of $\rho_{xx}(H)$ (the magnetoresistance, MR) at temperatures near 2 K. The data on the type and density of carriers were obtained from Hall effect measurements. Resistivity values were calculated from the measured resistance and the sample dimensions. For the magneto-transport experiment we used the “Hall bar” geometry, where the current was always applied perpendicular to the magnetic field direction.

III. RESULTS AND DISCUSSION

A. composition and structure

The grown crystals depicted on fig. 2 (a, b) are easily cleavable silvery flat needles of up to 0.5 cm in length and up to 0.1 cm in diameter with mass on the order of tens of milligrams. Crystals of TaIrTe$_4$ show a needle-like appearance, while TaRhTe$_4$ and Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ are more flattened, in a shape of thin stripes. As-grown crystals are extremely ductile and cleavable, even under regular handling operations. The results of the EDX confirm the nominal stoichiometry for TaRhTe$_4$ and TaIrTe$_4$ samples. Backscattered-electron SEM images (fig. 2 (c–e)) show uniform intensity, which is indicative of the absence of macroscopic inhomogeneities. Interestingly, the nominal ratio Ru:Ta=1:1 as-grown crystals in fact show Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ composition. This Ru:Ta ratio is consistent across different measurement points and different crystals, on natural and freshly cleaved surfaces, with a low EDX statistical error. Assuming the same connectivity in the structure as in TaIrTe$_4$ compound, this composition shift must manifest as structural modification hinted in [18]. This composition shift might be explained by the fact that Ru and Ta radii are quite close, resulting in e.g. mixing of the atoms in the same crystallographic position.

Results of EDX measurements on the TaIr$_{1-x}$Rh$_x$Te$_4$ are presented in table I. We see Rh/Ir substitution, with composition consistently shifted towards metal with the higher concentration.

For characterization of the structure powder x-ray diffraction (PXRD) was carried out including further analysis by Rietveld method. Results of the x-ray powder diffraction on TaRhTe$_4$ powdered crystals are presented in fig. 2 (f); PXRD patterns for Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ and TaIr$_{1-x}$Rh$_x$Te$_4$ are presented on fig. 10 in appendix, due to strong texture in both cases and high ductility in case of Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$. Rietveld analysis of those didn’t prove to be feasible. One observes fig. 2 diffraction shows broad reflections, which can be attributed to high ductility and ease of cleavage of the material. TaIrTe$_4$ was refined in the structural model presented in ICSD [18], (ICSD №73322, space group Pmn2$_1$). As reported by Mar et al. [18], we see that in case of TaRhTe$_4$ compound diffraction pattern is quite similar to TaIrTe$_4$. The TaRhTe$_4$ diffraction pattern was clearly indexed in Pmn2$_1$ space group, so for further Rietveld analysis we selected TaIrTe$_4$ as initial structure model, with Ir positions substituted by Rh with approximate lattice parameters extracted in the indexing step. Refinement in this model yielded lattice parameters of $a = 3.75670(11)$, $b = 12.5476(5)$, $c = 13.160(3)$ and cell volume of $V = 620.20(15)$ for TaRhTe$_4$. We observe small change of $a$
Magnetization ($10^{-4}$ emu Oe$^{-1}$ mol$^{-1}$) TaRhTe$_4$
Ta$_{1.25}$Ru$_{0.75}$Te$_4$

![Graph](Image)

FIG. 4. Temperature dependence of molar magnetization for TaRhTe$_4$ and Ta$_{1.25}$Ru$_{0.75}$Te$_4$. Inset: Curie-Weiss fit of paramagnetic contribution to Ta$_{1.25}$Ru$_{0.75}$Te$_4$.

and $c$ parameters $\Delta a \approx -0.03\AA$; $\Delta c \approx -0.03\AA$, and a considerable increase of $b$ ($\Delta b \approx 0.12\AA$) compared to the TaIrTe$_4$ structure. This can be explained by the smaller radius of the Rh atom, and as a result, might be indicative of tighter, and more extended zigzag chains in the structure. Refined atomic positions are presented in Table II. With that we can conclude that the TaRhTe$_4$ compound is isostructural to TaIrTe$_4$, which provides the opportunity to study change of physical properties with the change of lattice parameters and isovalent substitution.

SAED on individual TaTMTe$_4$ nanoflakes exfoliated from single crystals was performed to elaborate the crystallographic information obtained from the PXRD data reported in this work (Fig. 3). The SAED patterns for TaTMTe$_4$ acquired in [101] orientation are compared with simulated electron diffraction (ED) pattern using $Pmn2_1$ ($No.31$) space group. Here the [101] zone axis allows to distinguish lattice modulations in ternary TaTMTe$_4$ systems along $b$-direction in reciprocal space.

The good agreement of all symmetrical equivalent reflections in the ED patterns for TaIrTe$_4$ and TaRhTe$_4$ strongly suggest that these two crystals are isostructural and crystallize in $Pmn2_1$ space group as described in [18]. Interestingly, the Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_4$ electron diffraction patterns show that the unit cell of this compound is halved along $b$ compared to TaIrTe$_4$. To obtain a better fit with the SAED pattern we therefore used a crustal structure for Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_4$, which was derived from WTe$_2$ phase by filling the two W 2$a$ Wyckoff sites with Ta and Ru respectively. The proposed new structure matches nicely to the experimental SAED data of Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_4$, compound (purple dots, Fig. 3 d) and hence also provides a hint concerning the anomaly related to weak $k = 2$n + 1 reflections reported in [18]. Note, however, that this new structure does not reflect the large off-stoichiometry and the atomic positions and exact symmetry remain unclear as of now. Further studies are therefore required to fully resolve the Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_4$ structure.

B. Physical properties

1. Magnetization

For ternary compounds the temperature dependence of magnetization was measured. The derived temperature dependence of molar magnetization for TaRhTe$_4$ and Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_4$ is presented in fig. 4. All compounds exhibit diamagnetic behavior, with Curie-Weiss tails at low temperatures. Inset in Fig. 4 shows the Curie-Weiss analysis for Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_4$. Data confirms absence of any long range magnetic order down to 1.8 K.
emerging superconducting (SC) transition (see Fig. 9 in Appendix). Iridium doping of 8% the sample shows signatures of the superconducting state. Interestingly, for the intermediate Ir-doping of 8%, the sample shows signatures of the emerging superconducting (SC) transition (see Fig. 9 in Appendix).

3. Electronic structure calculations

We have performed calculations on the electronic structure within the DFT theory. The full relativistic generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof variant is used for the exchange correlation potential implemented in the full potential local orbital band-structure package (FPLO) [30, 31]. For the Brillouin zone (BZ) integration we used the tetrahedron method with 12×12×12k-mesh. The obtained electronic density of states (DOS) is presented in Fig. 7. The density of states decreases slightly at the Fermi level and then increases continuously similar to TaIrTe$_4$. Band structures of TaRhTe$_4$ with TaIrTe$_4$ are presented in Fig. 8. The main difference is appearance of the Rh-band close to the Fermi level.

2. Transport and magnetotransport

For stoichiometric TaRhTe$_4$ (Fig. 5) as well as for Ir-doped TaRh$_{1-x}$Ir$_x$Te$_4$ compound with $x = 0.08$ (Fig. 9) the temperature dependency of the diagonal resistivity in zero field flatten below $\approx 20$ K. In magnetic field, both for $B \parallel b$ and $B \parallel c$ (see Fig. 6), the resistivity also follows a classical almost isotropic quadratic dependence. The bulk carrier density determined from Hall resistance measurements (inset to Fig. 6) $n \approx 1.7 \times 10^{20}$ cm$^{-3}$ for the stoichiometric TaRhTe$_4$ by a factor of two lower compared to well investigated member of the family TaIrTe$_4$. As shown in Fig. 6, the resistivity of TaIrTe$_4$ varies quadratically with field which is quite similar in our case of TaRhTe$_4$. TaIrTe$_4$ resistivity exhibits a minor (8% at $B = 9$ T) anisotropy. The Hall resistivity $\rho_{xy}$ is negative and linearly grows with field, thus indicating dominant $n$-type electronic states with a similar bulk carrier density of $1.8 \times 10^{20}$ cm$^{-2}$. The initial minor anisotropy of the magnetoresistance becomes even lower upon doping with Rh or Ru.

Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ demonstrate metallic-type transport behavior (Fig. 5) at least down to 10 K. Although the resistivity shows a markedly different behavior at low temperatures, where it exhibits a minimum at $T \approx 9$ K, which appears to be a kink followed by a steep upturn while further lowering the temperature below 9 K. The origin of such non-monotonic resistivity remains unclear and requires further investigation.

The 22% substitution of Rh by Ir does not change significantly the resistivity $T$-dependence: RRR remains almost unchanged, whereas the carrier density increases by 34% to $2.3 \times 10^{20}$ cm$^{-3}$, and the magnetoresistance becomes fully isotropic. Interestingly, for the intermediate Ir-doping of 8%, the sample shows signatures of the emerging superconducting (SC) transition (see Fig. 9 in Appendix).

IV. CONCLUSION

In conclusion, we reported single crystal growth of layered van der Waals materials of the family TaTMTe$_4$ (TM=Ir,Rh,Ru), as well as several TaIr$_{1-x}$Rh$_x$Te$_4$ compounds. We confirmed the nominal compositions via SEM-EDX. In the Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ case we demonstrate that the compound is not stoichiometric with an actual composition of Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$. X-ray powder diffraction and further Rietveld refinement confirms that TaRhTe$_4$ is isostructural to TaIrTe$_4$ and crystallizes in non-centrosymmetric orthorhombic Pmn1 space group with a similar connectivity as WTe$_2$. SAED results indicate that Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ is a disordered analog of TaIrTe$_4$ structure type and further investigation of the structure is needed. Substitution series of TaIr$_{1-x}$Rh$_x$Te$_4$ were obtained for $x = 0.06; 0.14, 0.78, 0.92$ and we investigated magnetic and magnetotransport properties of the grown single crystals.

All samples have electronic ($n$-type) conduction. Any substitution of Rh or Ir was found to reduce mobility. All samples show weak MR field dependence. For the Rh series the MR is almost isotropic. Some compounds show a linear MR in low fields, atop of the parabolic one. Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ shows parabolic magnetoresistance which flattens out in high fields at the temperatures above 9 K. Magnetoresistance measurements below 9 K show a clear anomaly in fields below 5 T. We have performed electronic structure calculations using DFT for isostructural TaIrTe$_4$ and TaRhTe$_4$ together with the projected total density of states. The main difference is appearance of the Rh-band close to the Fermi level.

Due to the topological properties of the electronic band structure, the recent observation of the resistive switch-
We observed an indication of emerging superconductivity (SC) with critical temperature $T_c = 4$ K in TaRh$_{1-x}$Ir$_x$Te$_4$ compound for $x = 0.08$ and in TaIr$_{1-x}$Ru$_x$Te$_4$ for $x = 0.22$. As an example, we show in Fig. 9 the data for the former compound.

The inset in Fig. 9 zooms in a sharp drop of $\rho_{xx}(T)$ by 4 $\mu$ Ohm-cm both in zero field as temperature decreases below $T \approx 4$ K, and at $T = 2$ K as magnetic field decreases below 0.1 T. These features suggest that the drop of $\rho_{xx}$ is related with the SC transition at $T_c \approx 4$ K in zero field. Indeed, the transition temperature shifts to lower values as magnetic field increases, and the critical magnetic field decreases as temperature raises.

V. APPENDIX
FIG. 8. Band structure TaRhTe₄ vs TaIrTe₄ (a). Orbital contribution to the electronic band structure of TaRhTe₄ (b).

The zero-resistance state is not achieved, apparently because of a very small fraction of the superconducting state. In strong magnetic field, MR shows weak classical quadratic dependence, almost isotropic in θ. These slightly doped TaRh₁₋ₓIrₓTe₄ and TaIr(Ru)Te₄ samples, most likely, contain minor inclusions of several SC phases which emerge in a narrow interval of doping on the compound phase diagram. The interesting issue of potential superconductivity in these compounds requires additional more detailed studies.

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FIG. 9. (a) Temperature dependence of $\rho_{xx}$ for TaRh$_{0.92}$Ir$_{0.08}$Te$_4$. Inset shows low temperature region of $\rho_{xx}(T)$. (b) $\rho_{xx}$ versus magnetic field at two field orientations, measured at $T = 2$K. Inset: magnetic field dependence of the Hall resistivity $\rho_{xy}$. Arrows on panels (a) and (b) point at the onset of the SC transition; (c) low-field region of the $\rho_{xx}(H)$ dependencies measured at several fixed temperatures. (d) Low-temperature region of the $\rho_{xx}(T)$ dependencies measured at several field values at $T = 2$K.

FIG. 10. Powder x-ray diffraction patterns for TaIrTe$_4$, Ta$_{1.26(2)}$Ru$_{0.75(2)}$Te$_{4.000(8)}$ and TaIr$_{1-x}$Rh$_x$Te$_4$ ($x = 0.04$).

| Ir:Rh, nominal | EDX composition |
|----------------|-----------------|
| Ir$_{0.3}$Rh$_{0.1}$ | TaIr$_{0.96}$Rh$_{0.04}$Te$_4$ |
| Ir$_{0.7}$Rh$_{0.3}$ | TaIr$_{0.82}$Rh$_{0.14}$Te$_4$ |
| Ir$_{0.3}$Rh$_{0.7}$ | TaIr$_{0.22}$Rh$_{0.78}$Te$_4$ |
| Ir$_{0.2}$Rh$_{0.8}$ | TaIr$_{0.06}$Rh$_{0.92}$Te$_4$ |
| No | atom label | x   | y   | z   | Occ. | Site | Sym. |
|----|------------|-----|-----|-----|------|------|------|
| 1  | Ta         | 0.00000 | 0.05580 | -0.19200 | 1.000 | 2a   | m..  |
| 2  | Ta         | 0.00000 | 0.26530 | 0.29100 | 1.000 | 2a   | m..  |
| 3  | Rh         | 0.00000 | 0.52760 | -0.19800 | 1.000 | 2a   | m..  |
| 4  | Rh         | 0.00000 | 0.75430 | 0.33100 | 1.000 | 2a   | m..  |
| 5  | Te         | 0.00000 | 0.05945 | 0.19049 | 1.000 | 2a   | m..  |
| 6  | Te         | 0.00000 | 0.19454 | 0.62601 | 1.000 | 2a   | m..  |
| 7  | Te         | 0.00000 | 0.34483 | -0.09190 | 1.000 | 2a   | m..  |
| 8  | Te         | 0.00000 | 0.40783 | 0.44478 | 1.000 | 2a   | m..  |
| 9  | Te         | 0.00000 | 0.57274 | 0.19981 | 1.000 | 2a   | m..  |
| 10 | Te         | 0.00000 | 0.67725 | 0.65759 | 1.000 | 2a   | m..  |
| 11 | Te         | 0.00000 | 0.85038 | -0.07740 | 1.000 | 2a   | m..  |
| 12 | Te         | 0.00000 | 0.90438 | 0.46746 | 1.000 | 2a   | m..  |