Enhanced thermoelectric performance of heavy-fermion compounds YbTM$_2$Zn$_{20}$ ($TM = Co, Rh, Ir$) at low temperatures

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Thermoelectricity allows direct conversion between heat and electricity, providing alternatives for green energy technologies. Despite these advantages, for most materials the energy conversion efficiency is limited by the tendency for the electrical and thermal conductivity to be proportional to each other and the Seebeck coefficient to be small. Here we report counter examples, where the heavy fermion compounds YbTM$_2$Zn$_{20}$ ($TM = Co, Rh, Ir$) exhibit enhanced thermoelectric performance including a large power factor ($PF = 74$ $\mu$W/cm$^2$K$^2$; $TM = Ir$) and a high figure of merit ($ZT = 0.07$; $TM = Ir$) at 35 K. The combination of the strongly hybridized electronic state originating from the Yb $f$-electrons and the novel structural features (large unit cell and possible soft phonon modes) leads to high power factors and small thermal conductivity values. This demonstrates that with further optimization these systems could provide a platform for the next generation of low temperature thermoelectric materials.

INTRODUCTION

Efficient thermoelectric materials show a confluence between the opposing properties of being poor thermal conductors and good electrical conductors and supporting a large induced voltage in response to a temperature gradient (thermopower) (1). While electrical current is only carried by electrons, heat current is carried by both electrons and lattice vibrations (phonons). This necessitates that a useful material will feature mechanisms through which phonons are strongly scattered but electrical conduction remains unperturbed, i.e., the “phonon-glass, electron-crystal” concept (1). An effective way to accomplish this has been realized in materials with large cage-like voids in their atomic arrangement that can be filled with loosely bound heavy ions that scatter phonons as they “rattle” (2, 3). To maximize the thermopower, a material must have a large and rapidly changing density of states near the Fermi energy (4, 5). This is accomplished in some f-electron materials, where the Kondo effect results in strong hybridization between the narrow f-level band and the broad metallic conduction band. In these Kondo lattice systems, it is often seen that there is an anomalously large Seebeck coefficient that peaks in the vicinity of the Kondo coherence temperature, i.e., the temperature range where the emergent heavy Fermi liquid begins to form due to hybridization effects (6–9). On the basis of such features, strategies that combine soft lattice phonon modes and Kondo lattice effects have previously been pursued in a variety of systems, most notably the filled skutterudites and chemical/structural relatives, but only with limited success (10).

Motivated by these earlier studies, we synthesized high-purity single crystals of YbTM$_2$Zn$_{20}$ ($TM = Co, Rh, Ir$) to assess their thermoelectric properties. These materials were earlier reported to form in a cubic structure that includes large Zn polyhedrons that coordinate the Yb ions (11). Important features of this structure include its large unit cells, a cage-like covalent framework, and low coordination numbers for the constituent atoms, all of which suggest that they could be good candidates for thermoelectric applications (2, 3). The cage dimensions of YbTM$_2$Zn$_{20}$, defined as the longest distance between the two vertices in the cage frame, are around 6 Å, which is comparable to that of many filled skutterudites that show soft phonon modes (1, 12, 13). Earlier work also shows that these compounds exhibit heavy-fermion behavior that emerges from the Yb Kondo lattice. Evidence for this include (i) that they have large electronic Sommerfeld coefficients due to enhanced mass [also seen in effective mass determined from the de Haas–van Alphen (dHvA) experiment (14)] change carrier quasiparticles; (ii) that the Kadowaki-Woods ratio is obeyed, reinforcing the conclusion that the enhanced Sommerfeld coefficient is a property of an enhanced mass Fermi liquid; (iii) that the electrical transport and the magnetic susceptibility exhibit Kondo coherence peaks; and (iv) that tuning of the electronic state using applied pressure produces a phase diagram that conforms to expectations from the Doniach phase diagram (15–20). As TM evolves from Co$\rightarrow$Rh$\rightarrow$Ir, the Kondo coherence temperature increases from roughly 1 to 10 K (15, 18–20), suggesting that these materials would be expected to exhibit chemically tunable large thermopowers at low temperatures. More generally, other Yb-containing thermoelectric materials also show promising features at high temperatures for power generation applications (e.g., Yb$_{14}$MnSb$_{11}$) (21). Despite these attractive features, to our knowledge, there has been no investigation of the thermoelectric figure of merit of the 1-2-20 family of compounds.

Here, we report single-crystal x-ray diffraction (XRD) measurements and the temperature (T) dependence of the thermopower (S), electrical resistivity (\(\rho\)), heat capacity (\(C_p\)), thermal conductivity (\(\kappa\)), and thermoelectric figure of merit (\(ZT = S^2T/\rho\kappa\)) for this family of materials. Our XRD measurements reveal atomic displacement parameters to be around 0.01 Å for the Yb ions (Table 1). This value is relatively small, yet in the same order of magnitude, compared with that in other materials with soft lattice modes. The averaging of the anisotropic vibrational modes may play a role here (22). We also find that the lattice thermal conductivity (\(\kappa_{lv}\)) is strongly reduced by the soft lattice phonon modes, with values in the range of 2 to 5 W/m·K for all three compounds (minimized for the TM = Ir analog). The low-temperature \(\rho\) varies depending on the coherence temperature of the materials but is roughly similar for all three compounds, with values

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and is found to be large, considering that it is a low-temperature value, an enhanced value of \( S \). Single-crystal XRD results from fitting \( C_p \) on the combined Debye-Einstein model are in parentheses.

| Specimen             | YbCo\(_2\)Zn\(_20\) | YbRh\(_2\)Zn\(_20\) | YbIr\(_2\)Zn\(_20\) |
|----------------------|----------------------|----------------------|----------------------|
| Yb Wyckoff site      | 8a                   | 8a                   | 8a                   |
| Zn2 Wyckoff site     | 16c                  | 16c                  | 16c                  |
| Yb-\( 1\) (Å)        | 2.3295(3)            | 3.0633(1)            | 3.0662(1)            |
| Yb-\( 2\) (Å)        | 3.0873(4)            | 3.0994(3)            | 3.0928(4)            |
| Zn-\( 1\) (Å)        | 2.9589(3)            | 3.0075(3)            | 3.0059(4)            |
| Cage dimension (Å)   | 5.9113(4)            | 5.9549(4)            | 5.9515(5)            |
| \( U_{iso} \) of \( \text{Yb} \) (Å) | 0.00781(1)       | 0.00688(9)           | 0.00881(10)          |
| \( \theta_0\) (K)    | 329(265)             | 228(250)             | 224(240)             |
| \( \nu \) (m/s)      | 5.9549(4)            | 5.9549(4)            | 5.9515(5)            |
| \( A \) (10\(^{-12}\) s\(^{-1}\)) | 8.8                  | 12.4                 | 17.5                 |
| \( B \) (10\(^{-18}\) s K\(^{-1}\)) | 2.6                  | 0.7                  | 1.8                  |
| \( C \) (10\(^{13}\) s\(^{-2}\)) | 7.2                  | 17.6                 | 16                   |
| \( \epsilon_0 \) (THz) | 1.5                  | 1.9                  | 2.4                  |
| \( \theta_0 \) (K)   | 72(76)               | 91(95)               | 115(110)             |

Table 1. Structural diameters from single-crystal XRD and fitting parameters of \( \kappa \), using the Debye model as described in the text. The results from fitting \( C_p \) based on the combined Debye-Einstein model are in parentheses.

of 30 to 60 microhm-cm for \( 12 \leq T \leq 50 \) K. The Seebeck coefficient \( S \) exhibits a peak that is maximized for \( TM = \text{Ir} \) near 30 K at an enhanced value of \( -65 \mu V/K \). \( ZT \) is calculated from these quantities and is found to be large, considering that it is a low-temperature value, especially for YbIr\(_2\)Zn\(_20\) with a value of \( ZT = 0.07 \) at \( T = 35 \) K. This \( ZT \) value is nearly an order of magnitude larger than that of many competitive and well-known thermoelectric materials for cooling applications, particularly Bi\(_2\)Te\(_3\) (\( ZT \sim 0.008 \) at 35 K) and chemical analogs like CsBi\(_4\)Te\(_6\) (\( ZT \sim 0.01 \) at 35 K) (23). From this, we propose that YbTM\(_2\)Zn\(_20\) and the wider family of chemical analogs offer a long-desired stage upon which to develop a new generation of thermoelectric materials for low-temperature applications, e.g., for use in satellites or spacecraft and cryogenic cooling at temperatures below liquid nitrogen.

**RESULTS**

**Single-crystal XRD**

YbTM\(_2\)Zn\(_20\) (\( TM = \text{Co, Rh, Ir} \)) crystallizes in space group \( Fd-3m \) (#227) with \( Z = 8 \). Using the molten metal flux growth technique (17–19), we have obtained large single crystals of YbTM\(_2\)Zn\(_20\) (several millimeters in size). For example, Fig. 1A shows the as-synthesized YbCo\(_2\)Zn\(_20\) with the triangle face corresponding to the (111) crystallographic plane, indicating a [111] directional growth preference. Figure 1B shows the unit cell viewed along the [111] direction, suggesting a kagome lattice formed by the Yb and the transition metal atoms. Each Yb atom is surrounded by 16 Zn atoms and each \( TM \) is surrounded by 12 Zn atoms, thus forming two types of polyhedrons, Frank-Kasper polyhedron and icosahedron, respectively (Fig. 1C). The coordination between the Yb atoms and the \( TM-Zn \) cages is shown in Fig. 1 (D and E), where it is seen that there is no direct bonding between any Yb and TM atoms. For the Frank-Kasper polyhedron (Fig. 1F), the framework is formed by the 4 nearest neighbors (16c) and the 12 next nearest neighbors (96g) of the Zn atoms with Yb at the center. For this cluster, we define the cage dimension as the longest distance between the Zn atoms in the cage framework and list the diameters of the Frank-Kasper polyhedra in Table 1 (all are between 9.91 and 9.54 Å). The cage dimension changes slightly with the \( TM \) atoms, and the largest value was observed in YbRh\(_2\)Zn\(_20\), presumably because of the larger covalent radius of Rh compared to Co and Ir. Overall, the cage dimensions of YbTM\(_2\)Zn\(_20\) have values that are comparable to those of the Yb-filled skutterudite Yb\(_0.1\)CoSb\(_3\) and the skutterudite derivative Yb\(_{0.1}\)Co\(_2\)Ge\(_2\)Se\(_6\), where the Yb ions exhibit “ratting” behavior (24–26), suggesting that similar behavior might be expected here. Although the atomic displacement parameters are relatively small (~0.01 Å) for the Yb ions, evidence for soft lattice phonon modes are observed from both the temperature-dependent \( \kappa \) and the heat capacity (\( C_p \)), which will be discussed in the light of understanding the phonon transport in these materials.

**Thermoelectric property measurements**

Temperature-dependent Seebeck coefficient (\( S \)) measurements (gradient sweep method), four-probe resistivity (\( \rho \)) measurements, and steady-state thermal conductivity (\( \kappa \)) measurements from 12 to 300 K were performed for single crystals of YbTM\(_2\)Zn\(_20\) to characterize both \( PF \) and \( ZT \). The single crystals were carefully aligned before mounting so that both the thermal gradient and the electrical current were along the [100] crystallographic direction. Figure 2 shows \( S(T) \), where the low \( T \) values are large and negative. With increasing \( T \), there are breaks in slope near 50 K for \( TM = \text{Co and Rh} \), and a well-defined peak near 35 K for \( TM = \text{Ir} \), consistent with the earlier reported Kondo lattice behavior (6–9). Above the peak temperature, the absolute value of \( S \) decreases with increasing temperature, eventually changing sign from negative to positive at 185 and 240 K for YbCo\(_2\)Zn\(_20\) and YbRh\(_2\)Zn\(_20\), respectively, indicating that there is a competition between electrons and hole regarding the dominant charge carrier type. This is consistent with results from band structure calculations, which show both electron and hole pockets near the Fermi level (27). We also note that the \( S \) value of YbIr\(_2\)Zn\(_20\) remains negative up to 300 K but is estimated to have a crossover to positive values near 370 K. The inset of Fig. 2 shows \( \rho(T) \) for all three specimens. Similar behavior is seen between them, where \( \rho \) decreases with increasing temperature for \( 12 < T < 40 \) K and then increases, as expected from metallic transport. This is in agreement with earlier measurements, where the initial decrease seen here is the high temperature tail of a Kondo coherence peak that is centered at \( <10, 30, \) and \( 20 \) K for \( TM = \text{Co, Rh, and Ir} \) respectively (15–20). Note that the varying values of the coherence temperature are due to the different hybridization strengths between the three compounds (20). The combination of enhanced \( S \) values and the relatively low \( \rho \) at low \( T \) results in large peak values in the power factor (\( PF = S^2/\rho \)) of 7, 35, and 74 \( \mu W/cm-K^2 \) for YbCo\(_2\)Zn\(_20\), YbRh\(_2\)Zn\(_20\), and YbIr\(_2\)Zn\(_20\), respectively.

Because both electrical transport and thermal transport contribute to the efficiency of thermoelectricity, it is important to quantify the thermal properties of these compounds. To do this and to better understand the impact of the soft lattice phonon modes on the thermal
transport in these materials, we measured $C_p$ (Fig. 3) and $\kappa$ (Fig. 4) and estimated the Debye temperature ($\theta_D$), the Einstein temperature ($\theta_E$), and different phonon scattering parameters that represent the importance of different phonon scattering mechanisms. We first estimate $\theta_D$ from the $T^3$ dependence of $C_p$, to be 239, 228, and 224 K for YbCo$_2$Zn$_{20}$, YbRh$_2$Zn$_{20}$, and YbIr$_2$Zn$_{20}$, respectively (straight line fit in Fig. 3 insets). A more detailed fit that incorporates both the Debye and Einstein models is also shown in Fig. 3 and yields similar values (see Table 1) (28). We note that $C_p$ features a large electronic Sommerfeld coefficient at low temperature (insets of Fig. 3), just like what has been reported in earlier study, which suggests heavy-fermion behavior (7–9, 18–20). This result also corroborates with the large effective mass obtained from the dHvA experiment (14).

Figure 4A shows $\kappa$ from 12 to 300 K. Because of the large conventional unit cell (184 atoms per unit cell), the overall $\kappa$ is relatively low. Applying the Wiedemann-Franz law where $\kappa_L = L_0 \sigma T$ ($L_0$ is the Lorentz number), we obtain $\kappa_L$ as a function of temperature from $\kappa - \kappa_L$ (Fig. 4B). Because of the low $\rho$ values of YbTM$_2$Zn$_{20}$, $\kappa$ is dominated by $\kappa_L$ throughout the entire measured temperature range. The overall lower $\rho$ of YbCo$_2$Zn$_{20}$ compared with that of the other two systems, contributes to higher $\kappa_L$ and therefore to higher $\kappa$. After subtracting $\kappa_L$, $\kappa_1$ for all three systems is quite similar, as expected for compounds that share the same structure. To estimate the corresponding phonon scattering parameters, we used the Debye approximation to fit $\kappa_L$ (solid lines in Fig. 5B) using the expression (29)

$$\kappa_L = \frac{k_B}{2\pi^2\nu} \left( \frac{k_B T}{\nu} \right)^3 \int_0^{\nu/T} \frac{x^4 e^x}{\tau_C^4 (e^x - 1)^2} dx$$

where $x = h\omega/k_BT$ is dimensionless, $\nu$ is the speed of sound, and $\tau_C$ is the phonon scattering relaxation time. $\tau_C^{-1}$ can be further written as

$$\tau_C^{-1} = \frac{\nu}{L} + A\omega^4 + B\omega^2 T \exp \left( \frac{\theta_D}{3T} \right) + \frac{C\omega^2}{(\omega_0^2 - \omega^2)^2}$$

where $L$ is the grain size, $\omega$ is the phonon frequency, $\omega_0$ is the resonance frequency, and the coefficients $A$, $B$, and $C$ are fit parameters. The terms in Eq. 2 represent grain boundary phonon scattering, point defect phonon scattering, Umklapp scattering, and resonance scattering, respectively. In our fits, the $\nu$ values were calculated from the elastic constant reported in (16). The fit parameters were defined using a minimization of best sequence fit functions as compared to the experimental data and are listed in Table 1 together with the other related physical parameters. Excluding the transition elements, in each formula unit, the average mass of each atom is about 70 g/mol. As the transition element changes from Co to Rh and then Ir, the mass
The difference between TM and the average atomic mass of the unit cell increases. This creates enhanced mass fluctuation scattering between TM and the rest of the atoms in the unit cell, as indicated by the increased point defect phonon scattering parameter $A_T$. To quantitatively investigate the effect of the transition metals on $B$, information about the Grüneisen parameters would be required, so this analysis is not presented. The constant $\omega_0$ represents the rattling frequency of Yb atoms due to the dynamic disorder resonance, and from our fits, we obtain values of $\omega_0 \sim 2 \text{THz}$ for all three specimens. This is as expected, because all three specimens have a similar cage size. We note that the $\omega_0$ values of YbTM$_2$Zn$_{20}$ are similar to those of Yb$_{0.19}$Co$_{4}$Sb$_{12}$–Sn$_x$ ($x = 0, 0.05, \text{and} 0.2$), likely due to size similarity of the cages $(13)$. On the basis of $\omega_0$, we estimate Einstein temperatures $(\theta_E = h\omega_0/\kappa_B)$ to be 72, 91, and 115 K for YbCo$_2$Zn$_{20}$, YbRh$_2$Zn$_{20}$, and YbIr$_2$Zn$_{20}$, respectively. These values also agree quite well with the fitting results from $C_p$ by applying a combined Debye-Einstein model (Table 1). Thus, the $\kappa$ analysis shows that the cage-like structure, coupled with the soft lattice phonon modes, results in small $\kappa_L$ values. This directly contributes to the overall low $\kappa$, which is essential for good thermoelectric materials.

**DISCUSSION**

The large $PF$ values of YbTM$_2$Zn$_{20}$ compounds (Fig. 5A) and the small $\kappa$ values result in remarkably large $ZT$ values for all three compounds and across broad $T$ ranges, with a maximum near $ZT = 0.07$ at 35 K for YbIr$_2$Zn$_{20}$ (Fig. 5B). To our knowledge, this is only second to Bi$_1$–$x$Sb$_x$ ($ZT = 0.15$) $(30)$. For comparison, the insets of Fig. 5 (A and B) show $PF$ and $ZT$ at 35 K for several well-known thermoelectric materials: FeSb$_2$ $(31)$, Bi$_{0.5}$Sb$_{1.5}$Te$_3$ (thermoelectric material from Marlow industry), Bi$_2$Te$_3$ (thermoelectric material standard from the National Institute of Science and Technology), CsBi$_4$Te$_6$ $(23)$, and YbAl$_3$ $(32)$. The $ZT$ value of YbIr$_2$Zn$_{20}$ is about an order of magnitude higher than these materials. Although YbAl$_3$ has large $PF$ at low temperatures ($PF = 200$ at 35 K), due to the relatively large $\kappa$ values the $ZT$ value of YbAl$_3$ peaks with 0.04 at 100 K ($ZT = 0.017$ at 35 K) $(32)$. We note that not many materials have been investigated with a focus on the thermoelectric performance at low temperatures. Considering the bulk thermodynamic and electrical transport measurements, we classify these compounds as phonon-glass, electron-crystal materials. We understand this behavior as resulting from (i) the Kondo coherent f-electron lattice $(7–9, 18–20)$ that leads...
These approaches can be directly adapted to the 1-2-20 compounds as systems, achieved by modifying the soft lattice modes. In similar skutterudite glass region where the power factor has its peak value. From the electric applications. materials as the next-generation materials for low-temperature thermoelectric properties. In particular, we obtain a ZT value of 0.07 at 35 K for YbIr2Zn20 and a corresponding large PF. Having addressed that, in order for these materials to be interesting for device applications, the maximum cooling power will need to be improved. We also propose several different approaches to tune and further improve the thermoelectric properties of the 1-2-20 materials. Our results provide new momentum to the concept that heavy-fermion systems with cage-like structures are potentially promising for thermoelectric applications.

MATERIALS AND METHODS
Sample synthesis
The title compounds were synthesized by molten flux growth method. Yb chunks (99.9%, Ames Labs), Co ingots (99.99%, Alfa Aesar), Rh ingots (99.99%, Alfa Aesar), Ir ingots (99.99%, Alfa Aesar), and Zn shot (99.999%, Alfa Aesar) in an atomic ratio of Yb:TM:Zn (TM = Co, Rh, Ir) = 1:2:60 were loaded into 2-ml alumina crucibles and sealed under vacuum in quartz tubes. The quartz tubes were then heated to 1050°C at a rate of 50°C/hour, held at 1050°C for 24 hours, and then cooled to 700°C at a rate of 4°C/hour. At this temperature, the remaining flux was separated from the crystals by centrifugation. Multimillimeter-size single crystals were obtained.

Single-crystal XRD
YbTM2Zn20 single-crystals were characterized structurally by single-crystal XRD using an Oxford-Diffraction Xcalibur2 CCD system with graphite monochromated Mo Kα radiation. Data were collected using 0 scans with 1° frame widths to a resolution of 0.4 Å, equivalent to 2° ≈ 125°. Reflections were recorded, indexed, and corrected for absorption using the Oxford-Diffraction CRYSTALS PRO software (37), and subsequent structure determination and refinement were carried out using the single-crystal x-ray structure refinement and analysis software package CRYSTALS (38), with SUPERFLIP (39) phasing algorithm on F². The data quality allowed an unconstrained full matrix refinement against F² with anisotropic thermal displacement parameters for all atoms. The crystallographic information files have been deposited with the Inorganic Crystal Structure Database (ICSD CSD-434009, CSD-434010, and CSD-434011 for YbCo2Zn20, YbRh2Zn20, and YbIr2Zn20, respectively). Electron-dispersive spectroscopy analyses corroborated the stoichiometries obtained from the refinement results.
Transport property measurements

The single crystals of Yb7M2Zn20 were aligned on an Enraf-Nonius CAD-4 diffractometer along their [100] axis before being cut into rectangular slabs of 2 mm by 1 mm by 0.5 mm dimensions for temperature-dependent four-probe ρ, S (gradient sweep method), and steady-state κ measurements in the temperature range from 12 to 300 K. The crystals were mounted such that the current and thermal gradient were along the [100] direction. All the surfaces were polished using 3-μm grid diamond polishing paper to reduce surface radiation losses during the measurements. The measurements were carried out in a custom radiation-shielded vacuum probe with uncertainties of 4, 6, and 8% for ρ, S, and κ, respectively (40). Electrical contacts to the specimens were made using silver epoxy, and thermal contacts were made using Stycast epoxy.

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contributions: The crystals were grown by K.W. and characterized by J.N.N. K.W. performed the measurements with assistance from Y.L., K.-W.C., D.H., and D.E.G. Analyses of the results were done by K.W. and D.H. The manuscript was written by K.W. and R.E.B. with contributions from all authors. Competing interests: The authors declare that they have no competing interests. Data and materials availability: All data needed to evaluate the conclusions in the paper are present in the paper and/or the Supplementary Materials. Additional data related to this paper may be requested from the authors.

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