Multigap superconductivity in centrosymmetric and noncentrosymmetric rhenium-boron superconductors

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We report a comprehensive study of the centrosymmetric Re_3B and noncentrosymmetric Re_7B_3 superconductors. At a macroscopic level, their bulk superconductivity (SC), with $T_c = 5.1$ K (Re_3B) and 3.3 K (Re_7B_3), was characterized via electrical-resistivity, magnetization, and heat-capacity measurements, while their microscopic superconducting properties were investigated by means of muon-spin rotation and relaxation (μSR). In both Re_3B and Re_7B_3 the low-T zero-field electronic specific heat and the superfluid density (determined via transverse-field μSR) suggest a nodeless SC. Both compounds exhibit some features of multigap SC, as evidenced by the temperature-dependent upper critical fields $H_{c2}(T)$, as well as by electronic band-structure calculations. The absence of spontaneous magnetic fields below the onset of SC, as determined from zero-field μSR measurements, indicates a preserved time-reversal symmetry in the superconducting state of both Re_3B and Re_7B_3. Our results suggest that a lack of inversion symmetry and the accompanying antisymmetric spin-orbit coupling effects are not essential for the occurrence of multigap SC in these rhenium-boron compounds.

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I. INTRODUCTION

The possibility to host unconventional and topological superconductivity (SC) or to act as systems to realize Majorana fermions [1–11] has made noncentrosymmetric superconductors (NCSCs) one of the most investigated materials in recent times. In NCSCs, a lack of inversion symmetry implies that admixtures of spin-singlet and spin-triplet superconducting pairings are allowed [1–3]. This sets the scene for a variety of exotic properties, such as upper critical fields beyond the Pauli limit [12,13], nodes in the superconducting gap [14–17], and multigap SC [18]. More interestingly, by using the muon-spin relaxation (μSR) technique, time-reversal symmetry (TRS) breaking has been observed to occur in the superconducting state of selected weakly correlated NCSCs. These include CaPtAs [17], $LaNiC_2$ [19], La_7T_3 (T = transition metal) [20–22], Zr_3Ir [23], and ReT [24–27]. Except for CaPtAs, where TRS breaking and superconducting gap nodes coexist below T_c [17,28], in most other cases the superconducting properties resemble those of conventional superconductors, characterized by a fully opened energy gap. In general, the causes behind TRS breaking in these superconductors are not yet fully understood and remain an intriguing open question.

To clarify the issue, α-Mn-type ReT superconductors have been widely studied and demonstrated to show a superconducting state with broken TRS [24–27]. Our previous comparative μSR studies on Re-Mo alloys, covering four different crystal structures (including the noncentrosymmetric α-Mn type), revealed that the spontaneous magnetic fields occurring below T_c were observed only in elementary rhenium and in $Re_{0.88}Mo_{0.12}$ [27,29,30]. By contrast, TRS was preserved in the Re-Mo alloys with a lower Re content (below ~88%), independent of their centro- or noncentrosymmetric crystal structures [30]. Both elementary rhenium and $Re_{0.88}Mo_{0.12}$ adopting a simple centrosymmetric structure (hcp-Mg type) strongly suggests that a noncentrosymmetric structure is not essential in realizing TRS breaking in ReT superconductors. The μSR results for the Re-Mo family, as well as other α-Mn-type superconductors, e.g., $Mg_{10}Ir_{19}B_{16}$, $Nb_{0.5}Os_{0.5}$, Re_3W, and Re_3Ta [31–34], where TRS is preserved, clearly indicate that not only the Re presence but also its amount are crucial for the appearance and the extent of TRS breaking in ReT superconductors. How these results can be understood within a more general framework clearly requires further investigation.

Rhenium-boron compounds represent another suitable candidate system for studying the TRS breaking effects in the family of Re-based superconductors. Indeed, upon slight

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changes of the Re/B ratio, both centrosymmetric Re_3B (C-Re_3B) and noncentrosymmetric Re_7B_3 (NC-Re_7B_3) compounds can be synthesized [35], the latter adopting the same Th_7Fe_3-type structure as La_7T_3 superconductors [20–22], which frequently exhibit broken TRS in the superconducting state. Although selected properties of Re_3B and Re_7B_3 have been investigated by different techniques [36–38], their superconducting properties at a microscopic level, in particular, the superconducting order parameter, require further investigation.

In this paper, we report on a comprehensive study of the superconducting properties of Re_3B and Re_7B_3 carried out via electrical-resistivity, magnetization, heat-capacity, and muon-spin rotation and relaxation measurements, as well as by electronic band-structure calculations. Our endeavors serve a dual purpose. First, since La_7T_3 shows evidence of TRS breaking below T_c, it is of interest to establish whether the isostructural Re_7B_3 compound also displays similar features. Second, by systematically investigating the C-Re_3B and NC-Re_7B_3 superconductors, the previous findings regarding the ReT family can be extended also to other NCSC families, thus providing further insight into the open question of TRS breaking in NCSCs.

II. EXPERIMENTAL AND NUMERICAL METHODS

Polycrystalline rhenium-boron compounds were prepared by arc melting Re (99.99%, ChemPUR) and B (99.995%, ChemPUR) powders with different stoichiometric ratios in a high-purity argon atmosphere. To improve the homogeneity, samples were flipped and remelted several times and, finally, annealed at 800 °C for 2 weeks. The x-ray powder diffraction, measured using a Bruker D8 diffractometer with Cu $K\alpha$ radiation, confirmed the orthorhombic centrosymmetric structure of Re_3B (*Cmcm*, No. 63) and the hexagonal noncentrosymmetric structure of Re_7B_3 ($P6_3mc$, No. 186; see details in Fig. S1 in the Supplemental Material [39]). The magnetization, electrical-resistivity, and heat-capacity measurements were performed on Quantum Design magnetic property measurement system and physical property measurement system instruments, respectively. The bulk μSR measurements were carried out at the multipurpose surface-muon spectrometer (Dolly) of the Swiss muon source at Paul Scherrer Institut, Villigen, Switzerland. The μSR data were analyzed by means of the MUSRFIT software package [40].

The electronic band structures of Re_3B and Re_7B_3 were calculated via density functional theory (DFT), within the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof realization [41], as implemented in QUANTUM ESPRESSO [42,43]. The projector augmented wave pseudopotentials were adopted for the calculation [44,45]. Electrons belonging to the outer atomic configuration were treated as valence electrons, here corresponding to 15 electrons in Re ($5s^25p^65d^56s^2$) and 3 electrons in B ($2s^22p^1$). The kinetic energy cutoff was fixed to 55 Ry. For the self-consistent calculation, the Brillouin zone integration was performed on a Γ-centered mesh of 15 × 15 × 10 k points for Re_3B and 12 × 12 × 18 k points for Re_7B_3. Experimentally determined lattice constants and atom positions were used in both calculations.

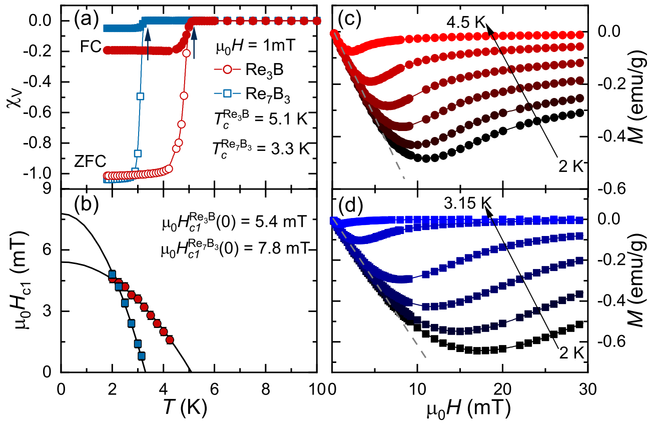

FIG. 1. (a) Temperature-dependent magnetic susceptibility of Re_3B and Re_7B_3, measured in an applied field of 1 mT using the ZFC and FC protocols. (b) Lower critical fields H_{c1} vs temperature. Solid lines are fits to $\mu_0H_{c1}(T) = \mu_0H_{c1}(0)[1-(T/T_c)^2]$. Field-dependent magnetization recorded at various temperatures for (c) Re_3B and (d) Re_7B_3. For each temperature, H_{c1} was determined as the value where $M(H)$ starts deviating from linearity (see dashed lines).

III. RESULTS AND DISCUSSION

The bulk superconductivity of C-Re_3B and NC-Re_7B_3 was first characterized by magnetic susceptibility measurements, using both field-cooled (FC) and zero-field-cooled (ZFC) protocols in an applied field of 1 mT. As indicated by the arrows in Fig. 1(a), a clear diamagnetic signal appears below the superconducting transition at $T_c = 5.1$ and 3.3 K for Re_3B and Re_7B_3, respectively. After accounting for the demagnetization factor, the superconducting shielding fraction of both samples is close to 100%, indicative of bulk SC, which was further confirmed by heat-capacity measurements [39]. To determine the lower critical field H_{c1}, essential for performing μSR measurements on type-II superconductors, the field-dependent magnetization $M(H)$ was collected at various temperatures. Some representative $M(H)$ curves are shown in Figs. 1(c) and 1(d) for Re_3B and Re_7B_3, respectively. The estimated H_{c1} values as a function of temperature are summarized in Fig. 1(b), resulting in $\mu_0H_{c1}(0) = 5.4(1)$ mT and 7.8(1) mT for Re_3B and Re_7B_3, respectively.

The upper critical field H_{c2} of Re_3B and Re_7B_3 was determined from measurements of the electrical resistivity, magnetization, and heat capacity under various magnetic fields up to 3 T (see Fig. S2 for details [39]). In zero magnetic field, the T_c values determined using different methods are highly consistent. The upper critical fields are summarized in Figs. 2(a) and 2(b) versus the reduced superconducting transition temperature $T_c/T_c(0)$ for Re_3B and Re_7B_3, respectively. $H_{c2}(T)$ was analyzed by means of Ginzburg-Landau (GL) [46], Werthamer-Helfand-Hohenberg (WHH) [47], and two-band (TB) models [48]. As shown in Fig. 2, both GL and WHH models can reasonably describe $H_{c2}(T)$ at low fields, i.e., $\mu_0H_{c2} < 0.5$ T (0.2 T) for Re_3B (Re_7B_3). However, at higher magnetic fields, both models deviate significantly from the experimental data and provide underestimated H_{c2} values. Such a discrepancy most likely hints at multiple superconducting gaps in Re_3B and Re_7B_3, as evidenced also by the

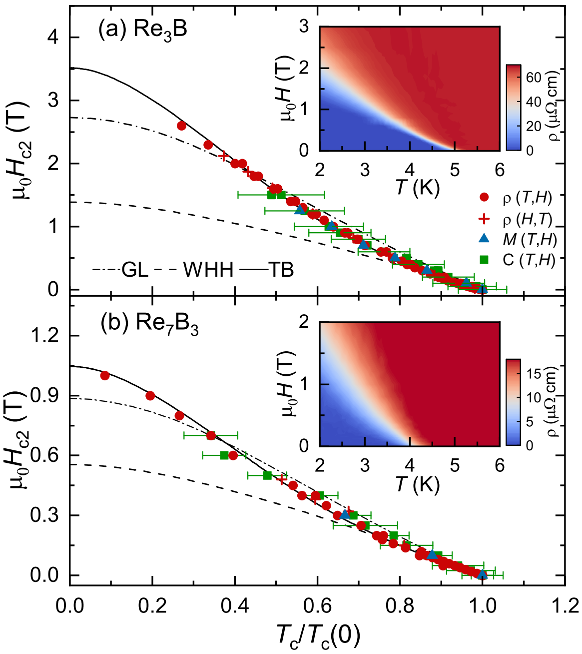

FIG. 2. Upper critical fields H_{c2} vs reduced temperature $T_c/T_c(0)$ for (a) Re_3B and (b) Re_7B_3, as determined from temperature-dependent electrical resistivity $\rho(T,H)$, magnetization $M(T,H)$, and heat capacity $C(T,H)$ and from field-dependent electrical resistivity $\rho(H,T)$. The contour plots of $\rho(T,H)$ in the insets indicate a clear positive curvature close to T_c. Three different models, including the GL (dash-dotted line), WHH (dashed line), and TB models (solid line), were used to analyze the $H_{c2}(T)$ data. Note the positive curvature visible near $\mu_0 H \sim 0.5$ and 0.2 T for Re_3B and Re_7B_3, respectively. The error bars refer to the superconducting transition widths ΔT_c in the specific-heat data.

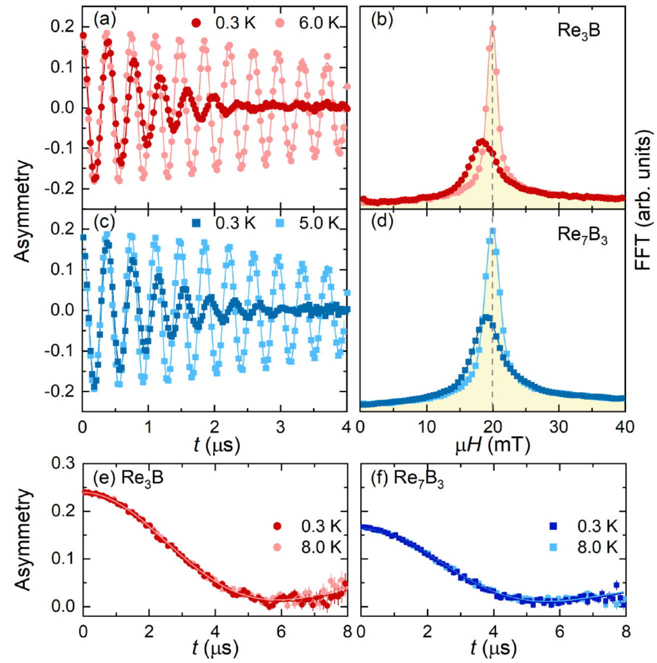

FIG. 3. (a) TF-μSR spectra of Re_3B collected in the superconducting (0.3 K) and normal (6 K) states in an applied magnetic field of 20 mT. (b) Fast Fourier transforms of the TF-μSR data shown in (a). (c) and (d) The analogous results for the Re_7B_3 case. The solid lines through the data are fits to Eq. (1), while the vertical dashed line marks the applied magnetic field. Note the clear diamagnetic shift and the field broadening at 0.3 K, as shown in (b) and (d). ZF-μSR spectra of (e) Re_3B and (f) Re_7B_3, collected in the superconducting and the normal states. Solid lines are fits using the equation described in the text. The overlapping data sets indicate no evident changes with temperature.

positive curvature of $H_{c2}(T)$, a typical feature of multigap superconductors, as e.g., $Lu_2Fe_3Si_5$ [49], MgB_2 [50,51], and the recently reported Mo_5PB_2 [52]. Physically, the positive curvature reflects the gradual suppression of the small superconducting gap upon increasing the magnetic field. As clearly demonstrated in the insets of Fig. 2, $H_{c2}(T)$ of Re_3B and Re_7B_3 exhibit clear kinks close to 0.5 and 0.2 T, respectively, most likely coinciding with the field values able to suppress the smaller gap. As shown by the solid lines in Fig. 2, the TB model shows remarkable agreement with the experimental data and provides $\mu_0 H_{c2}(0) = 3.5(1)$ and 1.05(5) T for Re_3B and Re_7B_3, respectively.

To investigate at a microscopic level the SC of Re_3B and Re_7B_3, we carried out systematic transverse-field (TF) μSR measurements in an applied field of 20 mT, i.e., more than twice their $\mu_0 H_{c1}(0)$ values [see Fig. 1(b)]. Representative TF-μSR spectra collected in the superconducting and normal states of Re_3B and Re_7B_3 are shown in Figs. 3(a) and 3(c), respectively. The additional field-distribution broadening due to the flux-line lattice (FLL) in the mixed state is clearly visible in Figs. 3(b) and 3(d), where the fast-Fourier transform (FFT) spectra of the corresponding TF-μSR data are presented. To describe the asymmetric field distribution (e.g., see FFT at 0.3 K), the TF-μSR spectra were modeled using

$$A(t) = \sum_{i=1}^{n} A_i \cos(\gamma_\mu B_i t + \phi) e^{-\sigma_i^2 t^2/2} + A_{bg} \cos(\gamma_\mu B_{bg} t + \phi). \tag{1}$$

Here A_i, A_{bg} and B_i, B_{bg} are the asymmetries and local fields sensed by implanted muons in the sample and sample holder (copper, which normally shows zero muon-spin depolarization), $\gamma_\mu/2\pi = 135.53$ MHz/T is the muon gyromagnetic ratio, ϕ is a shared initial phase, and σ_i is the Gaussian relaxation rate of the ith component. As shown by solid lines in Figs. 3(a) to 3(d), two oscillations (i.e., $n = 2$) are required to properly describe the TF-μSR spectra for both Re_3B and Re_7B_3. The derived $\sigma_i(T)$ as a function of temperature are summarized in the insets of Fig. 4. Above T_c, $\sigma_i(T)$ values are small and temperature independent, but below T_c they start to increase due to the onset of FLL and the increased superfluid density. Simultaneously, a diamagnetic field shift appears below T_c, given by $\Delta B(T) = \langle B \rangle - B_{appl.}$, where $\langle B \rangle = (A_1 B_1 + A_2 B_2)/A_{tot}$, $A_{tot} = A_1 + A_2$, with $B_{appl.}$ being the applied field. The effective Gaussian relaxation rate can be estimated from $\sigma_{eff}^2/\gamma_\mu^2 = \sum_{i=1}^{2} A_i[\sigma_i^2/\gamma_\mu^2 + (B_i - \langle B \rangle)^2]/A_{tot}$ [53]. Considering the constant nuclear relaxation rate σ_n in the narrow temperature range investigated here, confirmed also by zero-field (ZF) μSR measurements (see

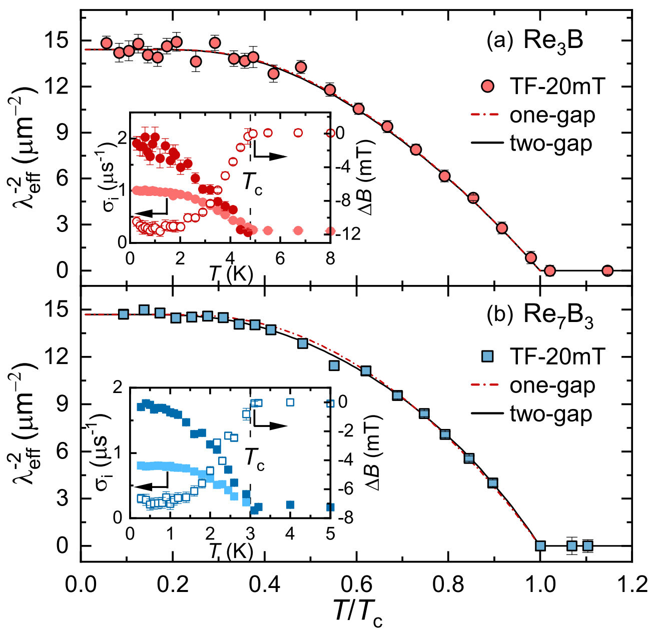

FIG. 4. Superfluid density vs reduced temperature T/T_c for (a) Re_3B and (b) Re_7B_3. The insets show the temperature-dependent muon-spin relaxation rate $\sigma_i(T)$ (left axis) and the diamagnetic shift $\Delta B(T)$ (right axis). The dashed lines in the insets indicate the T_c values, while the dash-dotted and solid lines in the main panels represent fits to a fully gapped *s*-wave model with one and two gaps, respectively.

details in Figs. 3(e) and 3(f) and Table S1 [39]), the superconducting contribution can be extracted using $\sigma_{sc} = \sqrt{\sigma_{eff}^2 - \sigma_n^2}$. Then, the effective magnetic penetration depth λ_{eff} and, thus the superfluid density ρ_{sc} ($\propto \lambda_{eff}^{-2}$) can be calculated following $\sigma_{sc} = 0.172\frac{\gamma_\mu \Phi_0}{2\pi}(1-h)[1+1.21(1-\sqrt{h})^3]\lambda_{eff}^{-2}$ [54,55], where $h = H_{appl}/H_{c2}$, with $\mu_0 H_{appl} = 20$ mT being the applied magnetic field.

We also performed ZF-μSR measurements in both the normal and the superconducting states of Re_3B and Re_7B_3. As shown in Figs. 3(e) and 3(f), neither coherent oscillations nor fast decays could be identified in the spectra collected above (8 K) and below T_c (0.3 K), hence implying the lack of any magnetic order or fluctuations. The weak muon-spin relaxation in the absence of an external magnetic field is mainly due to the randomly oriented nuclear moments, which can be modeled by means of a phenomenological relaxation function, consisting of a combination of Gaussian and Lorentzian Kubo-Toyabe relaxations [56,57], $A(t) = A_s[\frac{1}{3} + \frac{2}{3}(1-\sigma_{ZF}^2 t^2 - \Lambda_{ZF}t)e^{(-\frac{\sigma_{ZF}^2 t^2}{2} - \Lambda_{ZF}t)}] + A_{bg}$. Here A_s ($\equiv A_{tot}$) and A_{bg} are the same as in the TF-μSR case [see Eq. (1)]. σ_{ZF} and Λ_{ZF} represent the zero-field Gaussian and Lorentzian relaxation rates, respectively. As shown by the solid lines in Figs. 3(e) and 3(f), the derived relaxations in the normal and the superconducting states are almost identical (see Table S1) [39], as confirmed also by the practically overlapping ZF-μSR spectra above and below T_c. This lack of evidence for an additional μSR relaxation below T_c excludes a possible TRS breaking in the superconducting state of both C-Re_3B and NC-Re_7B_3.

The superfluid density ρ_{sc} vs the reduced T/T_c is shown in Figs. 4(a) and 4(b) for Re_3B and Re_7B_3, respectively. The temperature-independent superfluid density below $T_c/3$ hints a fully gapped SC in both cases. Therefore, we analyzed $\rho_{sc}(T)$ by means of a fully gapped *s*-wave model:

$$\rho_{sc}(T) = \frac{\lambda_{eff}^{-2}(T)}{\lambda_0^{-2}} = 1 + 2\int_{\Delta(T)}^{\infty} \frac{\partial f}{\partial E}\frac{E dE}{\sqrt{E^2 - \Delta^2(T)}}. \quad (2)$$

Here $f = (1 + e^{E/k_B T})^{-1}$ and $\Delta(T)$ are the Fermi- and the superconducting-gap functions. $\Delta(T)$ is assumed to follow $\Delta(T) = \Delta_0 \tanh\{1.82[1.018(T_c/T - 1)]^{0.51}\}$ [58], where Δ_0 is the superconducting gap at 0 K. Since the upper critical field $H_{c2}(T)$ exhibits typical features of multigap SC (see Fig. 2), the superfluid density was fitted using Eq. (2) with one and two gaps. In the two-gap case, $\rho_{sc}(T) = w\rho_{sc}^{\Delta^f}(T) + (1-w)\rho_{sc}^{\Delta^s}(T)$, with $\rho_{sc}^{\Delta^f}$ and $\rho_{sc}^{\Delta^s}$ being the superfluid densities related to the first (Δ^f) and second (Δ^s) gaps and w being a relative weight. For Re_3B, both the one- and two-gap models show an almost identical goodness-of-fit parameter ($\chi_r^2 \sim 1.2$), reflected in two practically overlapping fitting curves in Fig. 4(a). For Re_7B_3, instead, the two-gap model ($\chi_r^2 \sim 1.1$) is slightly superior to the one-gap model ($\chi_r^2 \sim 2.2$) [see Fig. 4(b)]. For the two-gap model, in the Re_3B case, the derived zero-temperature magnetic penetration depth is $\lambda_0 = 263(2)$ nm, and the gap values are $\Delta_0^f = 0.72(1)$ meV and $\Delta_0^s = 0.87(2)$ meV, with a weight $w = 0.7$. In the Re_7B_3 case, the corresponding values are $\lambda_0 =261(2)$ nm, $\Delta_0^f = 0.35(1)$ meV, and $\Delta_0^s = 0.57(2)$ meV, with $w = 0.27$. For the one-gap model, the gap values are $\Delta_0 = 0.77(2)$ and 0.50(2) meV for Re_3B and Re_7B_3, with the same λ_0 values as in the two-gap case.

Unlike in the clean-limit case [$\xi_0 \ll l_e$; see Eq. (2)], in the dirty limit, the BCS coherence length ξ_0 is much larger than the electronic mean-free path l_e. In the BCS approximation, the temperature-dependent superfluid density in the dirty limit is given by [59]

$$\rho_{sc}(T) = \frac{\Delta(T)}{\Delta_0}\tanh\left[\frac{\Delta(T)}{2k_B T}\right], \quad (3)$$

where $\Delta(T)$ is the same as in Eq. (2). For Re_3B, ξ_0 is larger than l_e ($\xi_0/l_e \sim 7.7$); therefore, Re_3B belongs to the dirty limit. However, in Re_7B_3, ξ_0 is smaller than l_e ($\xi_0/l_e \sim 0.3$); therefore, it belongs to the clean limit. For both compounds, ξ_0 and l_e are not significantly different and exhibit similar magnitudes. Hence, both Eqs. (2) and (3) describe quite well the low-T superfluid density and yield similar superconducting gaps (see Table I).

To further support the indications of a multigap SC obtained from H_{c2}, we measured also the zero-field specific heat down to $T_c/3$. After subtracting the phonon contribution ($\beta T^2 + \delta T^4$) from the measured data, the obtained electronic specific heat divided by γ_n, i.e., $C_e/\gamma_n T$, is shown in Figs. 5(a) and 5(b) vs the reduced temperature T/T_c for Re_3B and Re_7B_3, respectively. The superconducting-phase contribution to the entropy can be calculated following the BCS expression [59]:

$$S(T) = -\frac{6\gamma_n}{\pi^2 k_B}\int_0^{\infty}[f\ln f + (1-f)\ln(1-f)]\, d\epsilon, \quad (4)$$

TABLE I. Normal- and superconducting-state properties of C-Re_3B and NC-Re_7B_3, as determined from electrical-resistivity, magnetization, specific-heat, and μSR measurements, as well as from electronic band-structure calculations. The London penetration depth λ_L, the effective mass $m^\star$, carrier density n_s, BCS coherence length ξ_0, electronic mean free path l_e, Fermi velocity v_F, and effective Fermi temperature T_F were estimated following the methods in Ref. [30].

Property	Units	Re_3B	Re_7B_3
Space group		*Cmcm*	$P6_3mc$
Inversion center		Yes	No
ρ_0	$\mu\Omega$ cm	68.0	18.5
Residual resistivity ratio		1.9	5.8
T_c^ρ	K	5.2	3.5
T_c^χ	K	5.1	3.3
T_c^C	K	4.7	3.1
$T_c^{\mu SR}$	K	4.8	2.9
$\mu_0 H_{c1}$	mT	5.4(1)	7.8(1)
$\mu_0 H_{c2}$	T	3.5(1)	1.05(5)
γ_n	mJ/mol K^2	9.6(1)	21.5(2)
Θ_D	K	390(3)	440(5)
$N(\epsilon_F)^C$	states/eV f.u.	4.1(1)	9.1(1)
$N(\epsilon_F)^{DFT}$	states/eV f.u.	2.35	5.7
$\Delta_0(C)$	meV	0.75(2)	0.47(1)
$\Delta_0(\mu SR)^{clean}$	meV	0.77(2)	0.50(2)
$\Delta_0(\mu SR)^{dirty}$	meV	0.66(2)	0.44(1)
w		0.7	0.27
$\Delta_0^f(C)$	meV	0.69(2)	0.32(1)
$\Delta_0^s(C)$	meV	0.79(2)	0.50(1)
$\Delta_0^f(\mu SR)$	meV	0.72(1)	0.35(1)
$\Delta_0^s(\mu SR)$	meV	0.87(2)	0.57(2)
λ_0	nm	263(2)	261(2)
$\lambda_{GL}(0)$	nm	353(4)	259(2)
$\xi(0)$	nm	9.7(1)	17.7(4)
κ		36(1)	14.6(5)
λ_L	nm	90(5)	229(2)
l_e	nm	2.2(1)	22(1)
ξ_0	nm	17(1)	6.4(1)
ξ_0/l_e		7.7	0.3
$m^\star$	m_e	7.0(2)	10.4(1)
n_s	10^{28} m^{-3}	2.4(3)	0.56(1)
v_F	10^5 m s^{-1}	1.5(1)	0.61(1)
T_F	10^4 K	1.0(1)	0.25(1)

where f is the same as in Eq. (2). Then, the temperature-dependent electronic specific heat below T_c can be obtained from $C_e(T) = T\frac{dS(T)}{dT}$. The dash-dotted lines in Fig. 5 represent fits of an s-wave model with $\gamma_n = 9.6(1)$ and $21.5(2)$ mJ/mol K^2 and a single gap $\Delta_0 = 0.75(2)$ and 0.47(1) meV for Re_3B and Re_7B_3, respectively. For Re_7B_3, while the one-gap model reproduces the data for $T/T_c \gtrsim 0.5$, it deviates from them at lower temperatures, hence yielding a slightly larger $\chi_r^2 \sim 7.8$ than the two-gap model (see below). On the contrary, the two-gap model exhibits better agreement with the experimental data. The solid line in

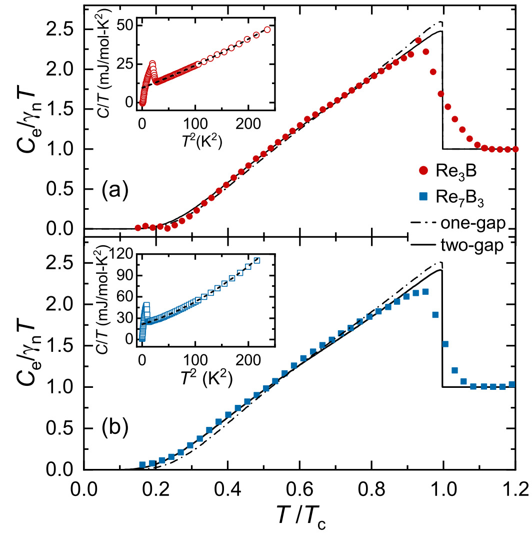

FIG. 5. Normalized electronic specific heat $C_e/\gamma_n T$ versus reduced temperature T/T_c for (a) Re_3B and (b) Re_7B_3. γ_n is the normal-state electronic specific-heat coefficient. The insets show the measured specific heat C/T versus T^2. The dashed lines in the insets are fits to $C/T = \gamma_n + \beta T^2 + \delta T^4$ for $T > T_c$, while the dash-dotted and solid lines in the main panel represent the electronic specific heat calculated by considering a fully gapped s-wave model with one and two gaps, respectively.

Fig. 5(b) is a fit with two energy gaps, i.e., $C_e(T)/T = wC_e^{\Delta^f}(T)/T + (1-w)C_e^{\Delta^s}(T)/T$. Here, each term represents a one-gap specific-heat contribution, with w, Δ^f, and Δ^s being the same parameters as in the case of superfluid density fits. In Re_7B_3, by sharing the w values, the two-gap model gives $\Delta_0^f = 0.32(1)$ meV and $\Delta_0^s = 0.50(1)$ meV, with $\chi_r^2 \sim 1.7$. Similarly, in Re_3B, the solid line in Fig. 5(a) is a fit with $\Delta_0^f = 0.69(2)$ meV and $\Delta_0^s = 0.79(2)$ meV. For Re_3B, although the two-gap model agrees slightly better with the experimental data for $T/T_c > 0.4$, below it, both one-gap and two-gap models deviate slightly from the measured data, probably reflecting an improper subtraction of the nuclear Schottky contribution (due to the limited lowest temperature that could be reached in this study; see details in Fig. S3 [39]). Measurements of zero-field specific heat down to the millikelvin range are clearly necessary to confirm the multigap nature of Re_3B and Re_7B_3. Note that, for both compounds, the superconducting parameters determined from the specific heat and the TF-μSR are remarkably consistent (see Table I).

Further evidence of the multigap SC and insight into the electronic properties of Re_3B and Re_7B_3 comes from band-structure calculations. The electronic band structures and the density of states (DOS) are shown in Fig. 6. As can be seen from Figs. 6(a) and 6(b), 4 and 12 different bands cross the Fermi level in Re_3B and Re_7B_3, respectively. Close to E_F, the DOS of both compounds is dominated by the Re 5d orbitals, while the contribution from the B 2p orbitals is negligible (see Figs. 6(a) and 6(b) and Fig. S4 [39]). Away from the Fermi level, the Re 5d and B 2p orbitals are highly hybridized. The estimated DOS at E_F are ~4.7 and ~11.4 states/(eV u.c.) for Re_3B and Re_7B_3, both comparable to the experimental values determined from the electronic specific-heat coefficient (see

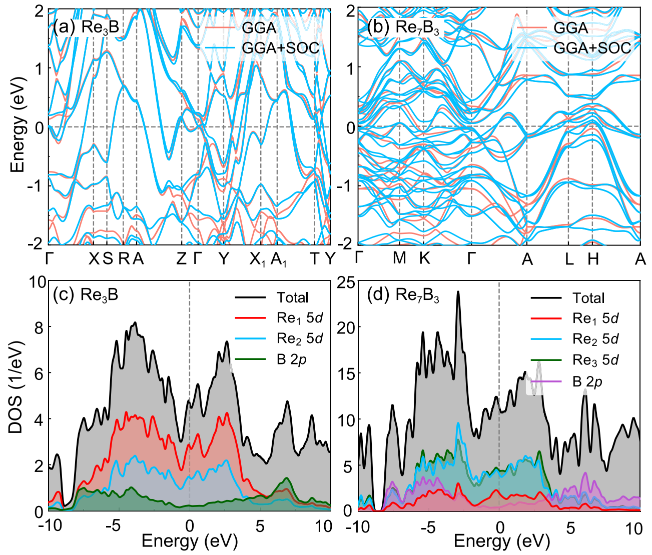

FIG. 6. Electronic band structure of C-Re_3B (a) and NC-Re_7B_3 (b), calculated by ignoring (red) and by considering (blue) the spin-orbit coupling. For both compounds, various bands which cross the Fermi level can be identified. The total and partial (Re $5d$ and B $2p$ orbitals) densities of states are shown in panels (c) and (d) for Re_3B and Re_7B_3, respectively.

Table I). We expect the multigap features of Re_3B and Re_7Be_3 to be closely related to the different site symmetries of Re atoms in the unit cell. For Re_3B, according to band-structure calculations, the contribution of Re1 ($8f$) atoms to the DOS is comparable to that of Re2 ($4c$) atoms [see Figs. 6(c)]. However, for Re_7B_3, the contributions of Re2 ($6c$) and Re3 ($6c$) atoms are preponderant compared to that of Re1 ($2b$) atoms.

Now, let us compare the superconducting parameters of Re_3B and Re_7B_3 with those of other superconductors. First, by using the SC parameters obtained from the measurements presented here, we calculated an effective Fermi temperature $T_F = 1.0(1) \times 10^4$ and $0.25(1) \times 10^4$ K for Re_3B and Re_7B_3 (see other parameters in Table I). T_F is proportional to $n_s^{2/3}/m^\star$, where n_s and $m^\star$ are the carrier density and the effective mass. Consequently, the different families of superconductors can be classified according to their T_c/T_F ratios into a so-called Uemura plot [60]. Several types of unconventional superconductors, including heavy fermions, organics, high-T_c iron pnictides, and cuprates, all lie in a $10^{-2} < T_c/T_F < 10^{-1}$ band (gray region in Fig. S5 [39]). Conversely, many conventional superconductors, as e.g., Al, Sn, and Zn, are located at $T_c/T_F \lesssim 10^{-4}$. Between these two categories lie several multigap superconductors, e.g., $LaNiC_2$, Nb_5Ir_3O, $ReBe_{22}$, $NbSe_2$, and MgB_2 [60–64]. Although there is no conclusive evidence for them to be classified as unconventional superconductors, the rhenium-boron superconductors lie clearly far off the conventional band. For Re_3B, $T_c/T_F = 4.8 \times 10^{-4}$ is almost identical to the analogous value for multigap $ReBe_{22}$ and $LaNiC_2$, the latter representing a typical example of NCSCs. However, for Re_7B_3, $T_c/T_F = 1.16 \times 10^{-3}$ is very close to the multigap Nb_5Ir_3O and elementary rhenium superconductors [27,30,63], the latter showing a breaking of TRS in the superconducting state and exhibiting a centrosymmetric crystal structure. In general, most of the weakly correlated NCSCs, e.g., ReT, Mo_3Al_2C, $Li_2(Pd, Pt)_3B$, and $LaNiC_2$, exhibit T_c/T_F values between the unconventional and conventional bands [64], and this is also the case for Re_7B_3.

Second, we discuss why the multigap feature is more prominent in Re_7B_3 than in Re_3B, both in the temperature-dependent superfluid density and in the zero-field electronic-specific data. In general, if the weight of the second gap is relatively small and the gap sizes are not significantly different, it is difficult to discriminate between single- and two-gap superconductors based on temperature-dependent superconducting properties. For Re_3B, the weight of the second gap $w = 0.3$ is similar to that of Re_7B_3 ($w = 0.27$). However, the gap sizes are clearly distinct in Re_7B_3 ($\Delta^f/\Delta^s \sim 0.6$) compared to Re_3B ($\Delta^f/\Delta^s \sim 0.9$). As a consequence, the multigap feature is more evident in Re_7B_3. On the other hand, from the analysis of $H_{c2}(T)$ using a two-band model, the derived interband and intraband couplings are $\lambda_{12} = 0.08$ and $\lambda_{11} \sim \lambda_{22} = 0.4$ and $\lambda_{12} = 0.01$ and $\lambda_{11} \sim \lambda_{22} = 0.15$ for Re_3B and Re_7B_3, respectively. In both cases, the interband coupling is much smaller than the intraband coupling. In addition, the interband coupling of Re_3B (0.08) is larger than that of Re_7B_3 (0.01). In such situation, the SC gaps open at different electronic bands, making the multigap features less distinguishable in the former case [65]. Despite these differences, the underlying multigap SC feature of both samples is reflected in their upper critical fields $H_{c2}(T)$ (see Fig. 2). To get further insight into the multigap SC of Re_3B and Re_7B_3, the measurements of the *field*-dependent superconducting Gaussian relaxation rate $\sigma_{sc}(H)$ and of the electronic-specific heat coefficient $\gamma(H)$ provide a possible alternative, with both data sets being expected to show a distinct field response compared to a single-gap superconductor [52,61]. For example, $\gamma(H)$ exhibits a clear change in slope when the applied magnetic field suppresses the small gap, a feature recognized as the fingerprint of multigap superconductors. Conversely, $\gamma(H)$ is mostly linear in the single-gap case.

Finally, we discuss the effects of the lack of inversion symmetry in Re_7B_3. In NCSCs, the occurrence of admixture of singlet and triplet pairings is allowed, whose mixing degree is generally believe to be related to the strength of the antisymmetric spin orbit coupling (ASOC) [1] and, thus, to unconventional SC. Here, by comparing NC-Re_7B_3 with C-Re_3B, we find that a noncentrosymmetric structure and its accompanying ASOC have little effect on the superconducting properties of Re_7B_3. First, the upper critical field of NC-Re_7B_3 is three times smaller than that of C-Re_3B; in both cases H_{c2} is well below the Pauli limit. Second, according to the ZF-μSR data (Fig. 3), TRS is preserved in the superconducting states of both samples. The results presented here further support the idea that the presence of rhenium and its amount are the two key factors which determine the appearance of TRS breaking in Re-based superconductors, while the noncentrosymmetric structure plays only a marginal role. Obviously, the Re content in both Re_3B and Re_7B_3 might be below a certain threshold value, e.g., 88% in Re-Mo alloys [30]. Therefore, it could be interesting to check, upon increasing the Re content, whether the TRS breaking effect will appear also in rhenium-boron superconductors and, if so, at which threshold value. Third, both Re_7B_3 and Re_3B exhibit nodeless SC with multiple gaps. In the case of Re_7B_3, whether the multigap feature is due to the band splitting caused by the ASOC or to the multiple bands crossing its Fermi level (the latter, in principle, accounting also for the C-Re_3B case) requires further theoretical work. Overall, as can be seen from Fig. 6(b), the ASOC and the band splitting are relatively small in Re_7B_3. Hence, we expect the spin-singlet pairing to be dominant in both the centrosymmetric and noncentrosymmetric rhenium-boron superconductors.

IV. CONCLUSION

To summarize, we studied the superconducting properties of the centrosymmetric Re_3B and noncentrosymmetric Re_7B_3 superconductors by means of electrical resistivity, magnetization, heat-capacity, and μSR techniques, as well as via numerical calculations. The superconducting states of Re_3B and Re_7B_3 are characterized by $T_c = 5.1$ and 3.3 K, and upper critical fields $\mu_0 H_{c2}(0) = 3.5$ and 1.05 T, respectively. The temperature-dependent zero-field electronic specific heat and superfluid density reveal a *nodeless* superconductivity, well described by an *isotropic s-wave* model. Both Re_3B and Re_7B_3 exhibit a positive curvature in their temperature-dependent upper critical field $H_{c2}(T)$, an established fingerprint of multigap superconductors. By combining our extensive experimental results with numerical band-structure calculations, we provided evidence of multigap superconductivity in both centro- and noncentrosymmetric rhenium-boron superconductors. Finally, the lack of spontaneous magnetic fields below T_c indicates that, unlike in ReT or elementary rhenium, the time-reversal symmetry is *preserved* in the superconducting state of both Re_3B and Re_7B_3. Our results suggest the spin-singlet paring channel to be dominant in rhenium-boron superconductors.

Note added. After the present manuscript was submitted, a related work by Sharma *et al.* [66] appeared, in which similar compounds were studied via the μSR technique.

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