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Redetermination of the crystal structures of rare-earth trirhodium diboride $RERh_3B_2$ (RE = Pr, Nd and Sm) from single-crystal X-ray data

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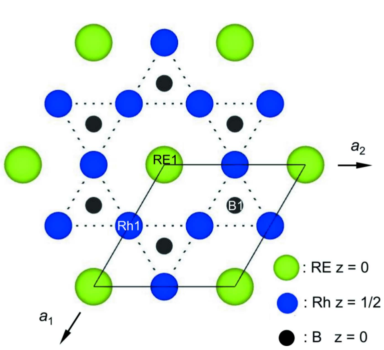
The crystal structures of the rare-earth (RE) trirhodium diborides praseodymium trirhodium diboride, $PrRh_3B_2$, neodymium trirhodium diboride, $NdRh_3B_2$, and samarium trirhodium diboride, $SmRh_3B_2$, were refined on the basis of single-crystal X-ray diffraction data. The crystal chemistry of $RERh_3B_2$ (RE: Pr, Nd, and Sm) compounds has previously been analyzed mainly on the basis of powder samples [Ku *et al.* (1980). *Solid State Commun*. **35**, 91–96], and no structural investigation by single-crystal X-ray diffraction has been reported so far. The crystal structures of the three hexagonal $RERh_3B_2$ compounds are isotypic with that of $CeRh_3B_2$; RE, Rh and B sites are situated on special positions with site symmetry $6/mmm$ (Wyckoff position $1a$), mmm ($3g$) and $\overline{6}m2$ ($2c$), respectively. In comparison with the previous powder X-ray study of hexagonal $RERh_3B_2$, the present redetermination against single-crystal X-ray data has allowed for the modeling of all atoms with anisotropic displacement parameters (ADPs). The ADPs of the Rh atom in each of the structures result in an elongated displacement ellipsoid in the direction of the stacking of the Rh kagomé-type layer. The features of obtained ADPs of atoms are discussed in relation to $RERh_3B_2$-type and analogous structures.



1. Chemical context

$CeCo_3B_2$-type $RERh_3B_2$ (RE = rare-earth element) compounds exhibit anomalous ferromagnetic properties (Malik *et al.*, 1983; Yamada *et al.*, 2004), and the unit-cell parameters of these compounds have been reported using powder X-ray diffraction (XRD) data (Ku *et al.*, 1980; Ku & Meisner, 1981). Higashi *et al.* (1987) analyzed the crystal structure of $CeRh_3B_2$ by using single-crystal XRD data and discussed the characteristics of the anisotropic atomic displacement parameters (ADP) of atoms in $CeRh_3B_2$ in relation to the structure. We report here the results of structural refinements using single crystals of $RERh_3B_2$ (RE = Pr, Nd, and Sm) grown by the arc-melting method.

2. Structural commentary

The crystal structures of hexagonal $RERh_3B_2$ (RE; La–Gd) compounds are isotypic with $CeCo_3B_2$ and crystallize in space-group type $P6/mmm$ (Kuz'ma *et al.*, 1969). The $CeCo_3B_2$ type of structure is ordered and can be derived from the $CaCu_5$ type of structure, whereby two distinct atoms (Rh and B) occupy the corresponding Cu sites. Each B atom is surrounded by six Rh atoms, forming a trigonal prism. Such $[BRh_6]$

trigonal prisms constitute a honeycomb structure and *RE* atoms are accommodated at the centers of the twelve [$RERh_{12}$] hexagonal prisms, as shown in Fig. 1. The $RERh_3B_2$ type of structure can also be described as being built up of kagomé layers of Rh atoms stacked along the *c* axis with an $\alpha\alpha$ stacking sequence and with B and *RE* atoms at the centers of the Rh triangular and hexagonal prisms, respectively.

The unit-cell parameters *a* and *c* and the unit-cell volume *V* of $RERh_3B_2$ (*RE* = La–Sm) compounds are shown in Fig. 2. The decrease in unit-cell volume results from the lanthanide contraction. The lattice parameters *a* and *c* decrease and increase, respectively. These anisotropic changes in the unit-cell parameters are consistent with those of a previous report using powder XRD analysis (Malik *et al.*, 1983).

The anisotropic change in the unit-cell parameters can be explained by the change in interatomic distances due to the lanthanide contraction. The ranges of B—Rh and *RE*—Rh distances are 2.2129 (1)–2.2151 (1) Å and 3.1370 (1)–3.1447 (1) Å (Table 1), respectively, which are close to the values of the sums of the atomic radii (r_{Rh} = 1.35 Å, r_B = 0.85 Å, r_{Pr} = 1.84 Å, r_{Nd} = 1.83 Å, and r_{Sm} = 1.81 Å; Daane *et al.*, 1954; Spedding *et al.*, 1956; Zachariasen, 1973). The *RE*—Rh interatomic distances decrease due to the effect of the lanthanoid contraction. Rh—Rh interatomic distances in the *ab* plane also decrease with a decrease in *RE*—Rh distances. By contrast, the Rh—Rh interatomic distances along the *c* axis increase. This causes the [$RERh_{12}$] hexagonal and [BRh_6] trigonal prisms to shrink horizontally and stretch vertically, resulting in decreases of the volumes of the hexagonal and trigonal prisms. Therefore, the unit-cells of $RERh_3B_2$ compounds change anisotropically, suggesting that the unit-cell changes elastically in response to the substitution of elements of different sizes at the *RE* site.

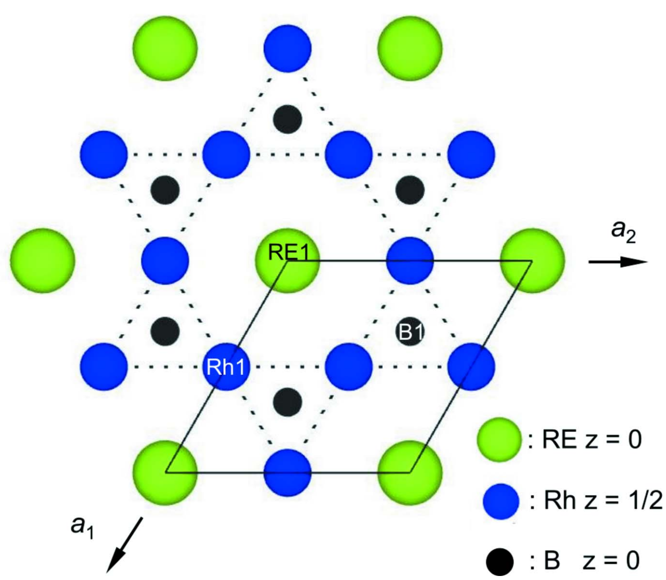


Figure 1
Structure of $RERh_3B_2$ compounds (space group: *P6/mmm*) as viewed along the *c* axis. B and *RE* atoms settle in the center of the trigonal and hexagonal prisms, respectively.

Table 1
Selected bond lengths (Å) in $RERh_3B_2$ (*RE* = Pr, Nd and Sm).

	$PrRh_3B_2$	$NdRh_3B_2$	$SmRh_3B_2$
RE—*RE* ×2	3.1084 (1)	3.1107 (1)	3.1190 (1)
RE—*RE* ×6	5.4676 (4)	5.4527 (3)	5.4438 (3)
RE—Rh ×12	3.1447 (1)	3.1388 (1)	3.1370 (1)
RE—B ×6	3.1557 (2)	3.1481 (1)	3.1430 (1)
B—Rh ×6	2.2151 (1)	2.2129 (1)	2.2140 (1)
B—B ×3	3.1084 (1)	3.1107 (1)	3.1190 (1)
B—B ×3	3.1567 (2)	3.1481 (1)	3.1430 (1)
Rh—Rh ×4	2.7338 (2)	2.7264 (1)	2.7219 (1)
Rh—Rh ×2	3.1084 (1)	3.1107 (1)	3.1190 (1)

The obtained ADPs for each atom are summarized in Table 2. The displacement ellipsoid of the Rh atom shows a larger anisotropy than those of the B and *RE* atoms, as shown in Fig. 3. The U_{33} of Rh atoms is approximately 2.1–2.6 times

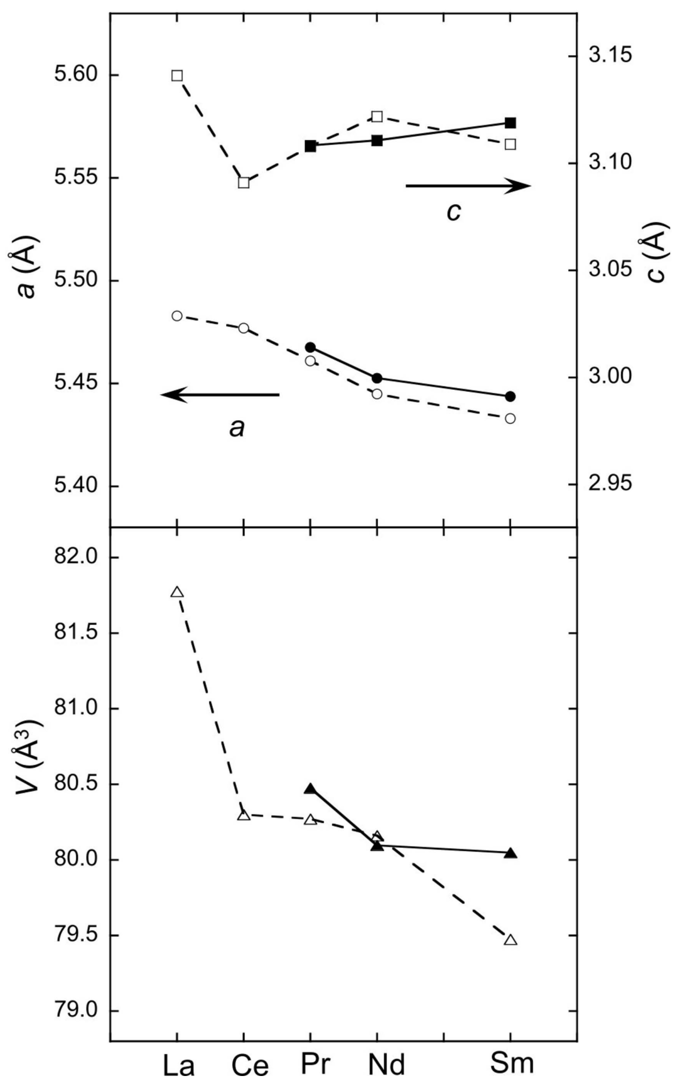


Figure 2
Unit-cell parameters *a* (circles), *c* (squares) and unit-cell volume (triangles) of $RERh_3B_2$ compounds. Closed and open marks refer to this study and previous work (Malik *et al.*, 1983), respectively.

Table 2
Atomic displacement parameters of *RE*, Rh, and B atoms in $RERh_3B_2$ (*RE* = Pr, Nd, and Sm).

Atom	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{eq} (10^{-3}Å^2)
$PrRh_3B_2$					
Pr	0.00861 (18)	0.00861	0.00780 (20)	0.00430 (9)	8.35 (1)
Rh	0.00495 (16)	0.00386 (18)	0.01040 (20)	0.00193 (9)	6.53 (1)
B	0.0095 (16)	0.0095	0.009 (2)	0.0048 (8)	9.3 (10)
$NdRh_3B_2$					
Nd	0.00896 (10)	0.00896	0.00662 (12)	0.00448 (5)	8.18 (9)
Rh	0.00492 (9)	0.00390 (11)	0.01104 (12)	0.00195 (5)	6.74 (8)
B	0.0100 (9)	0.0100	0.0079 (12)	0.0050 (4)	9.3 (6)
$SmRh_3B_2$					
Sm	0.00841 (12)	0.00841	0.00658 (14)	0.00420 (6)	7.80 (10)
Rh	0.00502 (11)	0.00389 (13)	0.01287 (14)	0.00194 (6)	7.39 (10)
B	0.0085 (10)	0.0085	0.0102 (15)	0.0043 (5)	9.1 (7)

larger than U_{11}, which means that the displacement ellipsoids of Rh atoms are elongated along the *c* axis. The displacement ellipsoids of Rh atoms with large anisotropy correspond to the anisotropic electric resistivity of $RERh_3B_2$ compounds (Yamada *et al.*, 2004; Obiraki *et al.*, 2006). The ADPs of *RE* atoms are described as displacement ellipsoids suppressed in the *c* axis ($U_{11} < U_{33}$). The feature of displacement ellipsoids of Rh and *RE* atoms is attributed to the unusually short *RE*—*RE* interatomic distances of 3.1084 (1)–3.1190 (1) Å, which are much shorter (15%) than the distance in the metal Pr, Nd, and Sm with hexagonal close-packed structures, (*i.e.*, 3.67, 3.66, and 3.62 Å, respectively). The short *RE*—*RE* interatomic distance is a common feature of the $CeCo_3B_2$ type of structure. Anisotropy of electric or thermal conductivity is also expected to be observed in $CeRh_3B_2$ compounds.

The obtained anisotropic ADPs of each atom in the structures of $RERh_3B_2$ compounds can be discussed in terms of the nucleation of interstitial atoms or layers in $PrRh_{4.8}B_2$ (Higashi *et al.*, 1988). Higashi *et al.* (1988) discovered a new layered structure, namely, $PrRh_{4.8}B_2$, which is regarded as a stacking variant of a modified $PrRh_3B_2$ structure. The interstitial single Rh layer is positioned between the Rh kagomé layers of the modified $PrRh_3B_2$ blocks. The displacement ellipsoid in the stacking direction of the Rh atom in the $PrRh_3B_2$ structure implies that the Rh kagomé layer in $PrRh_3B_2$ could be a base for the nucleation of interstitial atoms or layers. The appearance of disordered $La_{1-x}Rh_3B_2$ type and/or $Nd_{1-x}Rh_xRh_3B_2$ type of structures (Ohtani *et al.*, 1983; Vlasse *et al.*, 1983; Ku *et al.*, 1985) might be associated with the anisotropic ADPs of Rh and *RE* atoms.

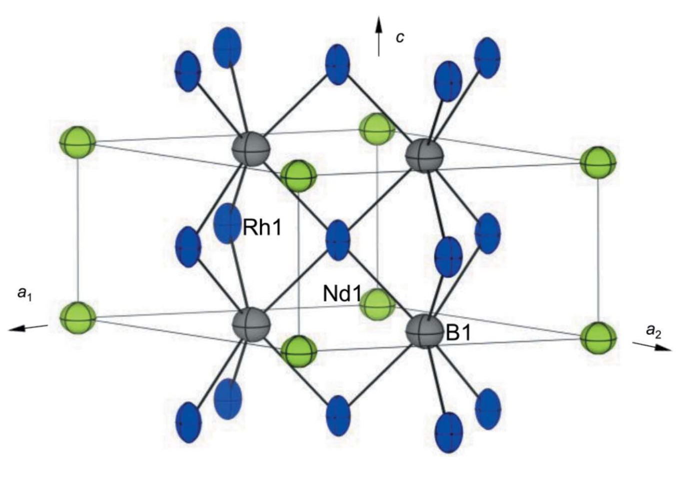


Figure 3
Displacement ellipsoids of each atom in $NdRh_3B_2$, with displacement ellipsoids drawn at the 99% probability level.

3. Synthesis and crystallization

$RERh_3B_2$ (*RE* = Pr, Nd, and Sm) single crystals were grown using the arc-melting method. The starting materials used were *RE* elements (99.9%), along with Rh (99.95%), and B (99.5%). They were weighed at an atomic ratio of (*RE*+3Rh+2B), and the mixtures of the starting materials were placed in an argon-arc melting furnace (ACM-01, Diavac). Each product was remelted three times to improve homogeneity. The grown crystals were composed of homogeneous $RERh_3B_2$, and the atomic ratio Rh/*RE* was confirmed to be 3.00 by energy dispersive X-ray spectroscopy.

4. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. A reciprocal space plot using all reflection data was in good agreement with the hexagonal lattice ($a \simeq 5$ Å and $c \simeq 3$ Å), and there was no evidence of superstructure reflections. The refinement was conducted under the assumption that the space group type was *P*6/*mmm*, as reported by Ku *et al.* (1980). Based on structural reports of $La_{1-x}Rh_3B_2$ and $Nd_{1-x}Rh_xRh_3B_2$, we determined whether Rh substitution and vacancies at the *RE* site were possible; however, the results were negative. Therefore, we concluded that the *RE* sites were completely occupied by *RE* elements. A correction for isotropic extinction was applied during the least-squares refinements. The final refinements were performed by applying anisotropic ADPs to each atom. The remaining electron densities located 0.7–0.6 Å around rhodium and *RE* heavy elements are censoring effects caused by the finite Fourier series.

Table 3
Experimental details.

	$PrRh_3B_2$	$NdRh_3B_2$	$SmRh_3B_2$
Crystal data			
M_r	471.26	474.59	480.70
Crystal system, space group	Hexagonal, *P*6/*mmm*	Hexagonal, *P*6/*mmm*	Hexagonal, *P*6/*mmm*
Temperature (K)	293	293	293
a, *c* (Å)	5.4676 (3), 3.10837 (16)	5.4527 (2), 3.11066 (13)	5.4438 (2), 3.11901 (12)
V (Å^3)	80.47 (1)	80.10 (1)	80.05 (1)
Z	1	1	1
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	29.43	30.57	32.61
Crystal size (mm)	0.05 × 0.03 × 0.03	0.05 × 0.05 × 0.02	0.06 × 0.05 × 0.02
Data collection			
Diffractometer	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Numerical (*CrysAlis PRO*; Rigaku OD, 2021)	Numerical (*CrysAlis PRO*; Rigaku OD, 2021)	Numerical (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.423, 0.601	0.424, 0.611	0.324, 0.542
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	733, 131, 126	827, 131, 130	696, 129, 128
R_{int}	0.017	0.010	0.011
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.909	0.908	0.907
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.053, 1.21	0.012, 0.032, 1.15	0.012, 0.032, 1.13
No. of reflections	131	131	129
No. of parameters	8	8	9
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.80, −1.18	0.97, −2.46	1.76, −0.97

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *VESTA* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

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Redetermination of the crystal structures of rare-earth trirhodium diboride *RE*Rh_3B_2 (*RE* = Pr, Nd and Sm) from single-crystal X-ray data

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Computing details

For all structures, data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Praseodymium trirhodium diboride (I)

Crystal data

$PrRh_3B_2$
M_r = 471.26
Hexagonal, *P*6/*mmm*
a = 5.4676 (3) Å
c = 3.10837 (16) Å
V = 80.47 (1) Å^3
Z = 1
$F(000)$ = 204
D_x = 9.724 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 623 reflections
θ = 4.3–39.9°
μ = 29.43 mm^{-1}
T = 293 K
Block, metallic
0.05 × 0.03 × 0.03 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: numerical (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.423, T_{max} = 0.601
733 measured reflections
131 independent reflections
126 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 40.3°, θ_{min} = 4.3°
$h = -9 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -3 \rightarrow 5$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.053
S = 1.21
131 reflections
8 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Pr1	0.000000	0.000000	0.000000	0.00835 (14)
Rh1	0.500000	0.000000	0.500000	0.00653 (13)
B1	0.333333	0.666667	0.000000	0.0093 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00861 (18)	0.00861 (18)	0.0078 (2)	0.00430 (9)	0.000	0.000
Rh1	0.00495 (16)	0.00386 (18)	0.0104 (2)	0.00193 (9)	0.000	0.000
B1	0.0095 (16)	0.0095 (16)	0.009 (2)	0.0048 (8)	0.000	0.000

Geometric parameters (Å, º)

Pr1—Pr1^{i}	3.1084 (2)	Pr1—Rh1^{x}	3.1447 (1)
Pr1—Pr1^{ii}	3.1084 (2)	Rh1—B1^{xi}	2.2151 (1)
Pr1—Rh1^{iii}	3.1447 (1)	Rh1—B1^{xii}	2.2151 (1)
Pr1—Rh1^{iv}	3.1447 (1)	Rh1—B1^{xiii}	2.2151 (1)
Pr1—Rh1	3.1447 (1)	Rh1—B1^{xiv}	2.2151 (1)
Pr1—Rh1^{v}	3.1447 (1)	Rh1—Rh1^{xv}	2.7338 (2)
Pr1—Rh1^{vi}	3.1447 (1)	Rh1—Rh1^{xvi}	2.7338 (2)
Pr1—Rh1^{vii}	3.1447 (1)	Rh1—Rh1^{iii}	2.7338 (2)
Pr1—Rh1^{viii}	3.1447 (1)	Rh1—Rh1^{xvii}	2.7338 (2)
Pr1—Rh1^{ix}	3.1447 (1)	Rh1—Rh1^{i}	3.1084 (2)
Pr1—Rh1^{ii}	3.1447 (1)	Rh1—Rh1^{ii}	3.1084 (2)
Pr1^{i}—Pr1—Pr1^{ii}	180.0	B1^{xiii}—Rh1—Rh1^{xv}	51.897 (2)
Pr1^{i}—Pr1—Rh1^{iii}	60.381 (1)	B1^{xiv}—Rh1—Rh1^{xv}	128.103 (2)
Pr1^{ii}—Pr1—Rh1^{iii}	119.619 (1)	B1^{xi}—Rh1—Rh1^{xvi}	128.103 (1)
Pr1^{i}—Pr1—Rh1^{iv}	119.619 (1)	B1^{xii}—Rh1—Rh1^{xvi}	51.897 (1)
Pr1^{ii}—Pr1—Rh1^{iv}	60.381 (1)	B1^{xiii}—Rh1—Rh1^{xvi}	128.103 (2)
Rh1^{iii}—Pr1—Rh1^{iv}	180.0	B1^{xiv}—Rh1—Rh1^{xvi}	51.897 (2)
Pr1^{i}—Pr1—Rh1	60.381 (2)	Rh1^{xv}—Rh1—Rh1^{xvi}	180.0
Pr1^{ii}—Pr1—Rh1	119.619 (2)	B1^{xi}—Rh1—Rh1^{iii}	51.896 (2)
Rh1^{iii}—Pr1—Rh1	51.528 (1)	B1^{xii}—Rh1—Rh1^{iii}	128.104 (2)
Rh1^{iv}—Pr1—Rh1	128.472 (1)	B1^{xiii}—Rh1—Rh1^{iii}	51.896 (2)
Pr1^{i}—Pr1—Rh1^{v}	119.619 (2)	B1^{xiv}—Rh1—Rh1^{iii}	128.104 (1)
Pr1^{ii}—Pr1—Rh1^{v}	60.381 (2)	Rh1^{xv}—Rh1—Rh1^{iii}	60.0
Rh1^{iii}—Pr1—Rh1^{v}	128.472 (1)	Rh1^{xvi}—Rh1—Rh1^{iii}	120.0
Rh1^{iv}—Pr1—Rh1^{v}	51.528 (1)	B1^{xi}—Rh1—Rh1^{xvii}	128.104 (2)

Rh1—Pr1—Rh1^{v}	180.0	B1^{xii}—Rh1—Rh1^{xvii}	51.896 (2)
Pr1^{i}—Pr1—Rh1^{vi}	60.381 (2)	B1^{xiii}—Rh1—Rh1^{xvii}	128.104 (2)
Pr1^{ii}—Pr1—Rh1^{vi}	119.619 (2)	B1^{xiv}—Rh1—Rh1^{xvii}	51.896 (2)
Rh1^{iii}—Pr1—Rh1^{vi}	51.528 (1)	Rh1^{xv}—Rh1—Rh1^{xvii}	120.0
Rh1^{iv}—Pr1—Rh1^{vi}	128.472 (1)	Rh1^{xvi}—Rh1—Rh1^{xvii}	60.0
Rh1—Pr1—Rh1^{vi}	97.678 (2)	Rh1^{iii}—Rh1—Rh1^{xvii}	180.0
Rh1^{v}—Pr1—Rh1^{vi}	82.322 (2)	B1^{xi}—Rh1—Rh1^{i}	45.442 (2)
Pr1^{i}—Pr1—Rh1^{vii}	119.619 (2)	B1^{xii}—Rh1—Rh1^{i}	134.558 (2)
Pr1^{ii}—Pr1—Rh1^{vii}	60.381 (2)	B1^{xiii}—Rh1—Rh1^{i}	134.558 (2)
Rh1^{iii}—Pr1—Rh1^{vii}	128.472 (1)	B1^{xiv}—Rh1—Rh1^{i}	45.442 (2)
Rh1^{iv}—Pr1—Rh1^{vii}	51.528 (1)	Rh1^{xv}—Rh1—Rh1^{i}	90.0
Rh1—Pr1—Rh1^{vii}	82.322 (2)	Rh1^{xvi}—Rh1—Rh1^{i}	90.0
Rh1^{v}—Pr1—Rh1^{vii}	97.678 (2)	Rh1^{iii}—Rh1—Rh1^{i}	90.0
Rh1^{vi}—Pr1—Rh1^{vii}	180.0	Rh1^{xvii}—Rh1—Rh1^{i}	90.0
Pr1^{i}—Pr1—Rh1^{viii}	60.381 (2)	B1^{xi}—Rh1—Rh1^{ii}	134.558 (2)
Pr1^{ii}—Pr1—Rh1^{viii}	119.619 (2)	B1^{xii}—Rh1—Rh1^{ii}	45.442 (2)
Rh1^{iii}—Pr1—Rh1^{viii}	120.763 (4)	B1^{xiii}—Rh1—Rh1^{ii}	45.442 (2)
Rh1^{iv}—Pr1—Rh1^{viii}	59.238 (4)	B1^{xiv}—Rh1—Rh1^{ii}	134.558 (2)
Rh1—Pr1—Rh1^{viii}	97.678 (3)	Rh1^{xv}—Rh1—Rh1^{ii}	90.0
Rh1^{v}—Pr1—Rh1^{viii}	82.322 (3)	Rh1^{xvi}—Rh1—Rh1^{ii}	90.0
Rh1^{vi}—Pr1—Rh1^{viii}	97.678 (3)	Rh1^{iii}—Rh1—Rh1^{ii}	90.0
Rh1^{vii}—Pr1—Rh1^{viii}	82.322 (3)	Rh1^{xvii}—Rh1—Rh1^{ii}	90.0
Pr1^{i}—Pr1—Rh1^{ix}	119.619 (2)	Rh1^{i}—Rh1—Rh1^{ii}	180.0
Pr1^{ii}—Pr1—Rh1^{ix}	60.381 (2)	B1^{xi}—Rh1—Pr1	110.289 (2)
Rh1^{iii}—Pr1—Rh1^{ix}	59.238 (4)	B1^{xii}—Rh1—Pr1	69.711 (3)
Rh1^{iv}—Pr1—Rh1^{ix}	120.763 (4)	B1^{xiii}—Rh1—Pr1	69.710 (2)
Rh1—Pr1—Rh1^{ix}	82.322 (3)	B1^{xiv}—Rh1—Pr1	110.290 (2)
Rh1^{v}—Pr1—Rh1^{ix}	97.678 (3)	Rh1^{xv}—Rh1—Pr1	115.764 (1)
Rh1^{vi}—Pr1—Rh1^{ix}	82.322 (3)	Rh1^{xvi}—Rh1—Pr1	64.236 (1)
Rh1^{vii}—Pr1—Rh1^{ix}	97.678 (3)	Rh1^{iii}—Rh1—Pr1	64.236 (1)
Rh1^{viii}—Pr1—Rh1^{ix}	180.0	Rh1^{xvii}—Rh1—Pr1	115.764 (1)
Pr1^{i}—Pr1—Rh1^{ii}	119.619 (2)	Rh1^{i}—Rh1—Pr1	119.619 (1)
Pr1^{ii}—Pr1—Rh1^{ii}	60.381 (2)	Rh1^{ii}—Rh1—Pr1	60.381 (2)
Rh1^{iii}—Pr1—Rh1^{ii}	82.322 (3)	B1^{xi}—Rh1—Pr1^{xviii}	69.711 (2)
Rh1^{iv}—Pr1—Rh1^{ii}	97.678 (3)	B1^{xii}—Rh1—Pr1^{xviii}	110.289 (3)
Rh1—Pr1—Rh1^{ii}	59.238 (4)	B1^{xiii}—Rh1—Pr1^{xviii}	110.290 (2)
Rh1^{v}—Pr1—Rh1^{ii}	120.762 (4)	B1^{xiv}—Rh1—Pr1^{xviii}	69.710 (2)
Rh1^{vi}—Pr1—Rh1^{ii}	128.472 (1)	Rh1^{xv}—Rh1—Pr1^{xviii}	64.236 (1)
Rh1^{vii}—Pr1—Rh1^{ii}	51.528 (1)	Rh1^{xvi}—Rh1—Pr1^{xviii}	115.764 (1)
Rh1^{viii}—Pr1—Rh1^{ii}	128.472 (1)	Rh1^{iii}—Rh1—Pr1^{xviii}	115.764 (1)
Rh1^{ix}—Pr1—Rh1^{ii}	51.528 (1)	Rh1^{xvii}—Rh1—Pr1^{xviii}	64.236 (1)
Pr1^{i}—Pr1—Rh1^{x}	60.381 (2)	Rh1^{i}—Rh1—Pr1^{xviii}	60.381 (2)
Pr1^{ii}—Pr1—Rh1^{x}	119.619 (2)	Rh1^{ii}—Rh1—Pr1^{xviii}	119.619 (2)
Rh1^{iii}—Pr1—Rh1^{x}	97.678 (3)	Pr1—Rh1—Pr1^{xviii}	180.0
Rh1^{iv}—Pr1—Rh1^{x}	82.322 (3)	Rh1^{xix}—B1—Rh1^{xx}	138.257 (2)
Rh1—Pr1—Rh1^{x}	120.762 (4)	Rh1^{xix}—B1—Rh1^{vi}	89.116 (4)
Rh1^{v}—Pr1—Rh1^{x}	59.238 (4)	Rh1^{xx}—B1—Rh1^{vi}	76.206 (4)
Rh1^{vi}—Pr1—Rh1^{x}	51.528 (1)	Rh1^{xix}—B1—Rh1^{xxi}	76.206 (4)

$Rh1^{vii}—Pr1—Rh1^{x}$	128.472 (1)	$Rh1^{xx}—B1—Rh1^{xxi}$	89.116 (4)
$Rh1^{viii}—Pr1—Rh1^{x}$	51.528 (1)	$Rh1^{vi}—B1—Rh1^{xxi}$	138.257 (2)
$Rh1^{ix}—Pr1—Rh1^{x}$	128.472 (1)	$Rh1^{xix}—B1—Rh1^{iii}$	138.257 (2)
$Rh1^{ii}—Pr1—Rh1^{x}$	180.0	$Rh1^{xx}—B1—Rh1^{iii}$	76.206 (4)
$B1^{xi}—Rh1—B1^{xii}$	180.0	$Rh1^{vi}—B1—Rh1^{iii}$	76.206 (4)
$B1^{xi}—Rh1—B1^{xiii}$	89.116 (4)	$Rh1^{xxi}—B1—Rh1^{iii}$	138.257 (2)
$B1^{xii}—Rh1—B1^{xiii}$	90.884 (4)	$Rh1^{xix}—B1—Rh1^{ix}$	76.206 (4)
$B1^{xi}—Rh1—B1^{xiv}$	90.884 (4)	$Rh1^{xx}—B1—Rh1^{ix}$	138.257 (2)
$B1^{xii}—Rh1—B1^{xiv}$	89.116 (4)	$Rh1^{vi}—B1—Rh1^{ix}$	138.257 (2)
$B1^{xiii}—Rh1—B1^{xiv}$	180.0	$Rh1^{xxi}—B1—Rh1^{ix}$	76.206 (4)
$B1^{xi}—Rh1—Rh1^{xv}$	51.897 (1)	$Rh1^{iii}—B1—Rh1^{ix}$	89.116 (4)
$B1^{xii}—Rh1—Rh1^{xv}$	128.103 (1)		

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*, *y*, *z*−1; (iii) −*x*+*y*+1, −*x*+1, *z*; (iv) −*x*+*y*, −*x*, *z*−1; (v) *x*−1, *y*, *z*−1; (vi) −*y*, *x*−*y*, *z*; (vii) −*y*, *x*−*y*−1, *z*−1; (viii) −*x*+*y*, −*x*, *z*; (ix) −*x*+*y*+1, −*x*+1, *z*−1; (x) *x*−1, *y*, *z*; (xi) −*x*+1, −*y*+1, −*z*+1; (xii) *x*, *y*−1, *z*; (xiii) −*x*+1, −*y*+1, −*z*; (xiv) *x*, *y*−1, *z*+1; (xv) −*y*+1, *x*−*y*, *z*; (xvi) −*y*, *x*−*y*−1, *z*; (xvii) −*x*+*y*+1, −*x*, *z*; (xviii) *x*+1, *y*, *z*+1; (xix) −*y*, *x*−*y*, *z*−1; (xx) *x*, *y*+1, *z*; (xxi) *x*, *y*+1, *z*−1.

Neodymium trirhodium diboride (II)

Crystal data

$NdRh_3B_2$
M_r = 474.59
Hexagonal, *P*6/*mmm*
a = 5.4527 (2) Å
c = 3.11066 (13) Å
V = 80.10 (1) Å^3
Z = 1
F(000) = 205
D_x = 9.839 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 729 reflections
θ = 4.3–40.7°
μ = 30.57 mm^{-1}
T = 293 K
Block, metallic
0.05 × 0.05 × 0.02 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: numerical (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.424, T_{max} = 0.611
827 measured reflections
131 independent reflections
130 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
θ_{max} = 40.2°, θ_{min} = 4.3°
h = −9→8
k = −7→9
l = −3→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.012
$wR(F^2)$ = 0.032
S = 1.15
131 reflections
8 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −2.46 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Nd1	0.000000	0.000000	0.000000	0.00818 (9)
Rh1	0.500000	0.000000	0.500000	0.00674 (8)
B1	0.333333	0.666667	0.000000	0.0093 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00896 (10)	0.00896 (10)	0.00662 (12)	0.00448 (5)	0.000	0.000
Rh1	0.00492 (9)	0.00390 (11)	0.01104 (12)	0.00195 (5)	0.000	0.000
B1	0.0100 (9)	0.0100 (9)	0.0079 (12)	0.0050 (4)	0.000	0.000

Geometric parameters (Å, º)

Nd1—Nd1^{i}	3.1107 (1)	Nd1—Rh1^{ii}	3.1388 (1)
Nd1—Nd1^{ii}	3.1107 (1)	Rh1—B1^{xi}	2.2129 (1)
Nd1—Rh1^{iii}	3.1388 (1)	Rh1—B1^{xii}	2.2129 (1)
Nd1—Rh1^{iv}	3.1388 (1)	Rh1—B1^{xiii}	2.2129 (1)
Nd1—Rh1^{v}	3.1388 (1)	Rh1—B1^{xiv}	2.2129 (1)
Nd1—Rh1^{vi}	3.1388 (1)	Rh1—Rh1^{xv}	2.7264 (1)
Nd1—Rh1	3.1388 (1)	Rh1—Rh1^{xvi}	2.7264 (1)
Nd1—Rh1^{vii}	3.1388 (1)	Rh1—Rh1^{iii}	2.7264 (1)
Nd1—Rh1^{viii}	3.1388 (1)	Rh1—Rh1^{xvii}	2.7264 (1)
Nd1—Rh1^{ix}	3.1388 (1)	Rh1—Rh1^{i}	3.1107 (1)
Nd1—Rh1^{x}	3.1388 (1)	Rh1—Rh1^{ii}	3.1107 (1)
Nd1^{i}—Nd1—Nd1^{ii}	180.0	B1^{xiii}—Rh1—Rh1^{xv}	51.974 (1)
Nd1^{i}—Nd1—Rh1^{iii}	60.296 (1)	B1^{xiv}—Rh1—Rh1^{xv}	128.026 (1)
Nd1^{ii}—Nd1—Rh1^{iii}	119.704 (1)	B1^{xi}—Rh1—Rh1^{xvi}	128.026 (1)
Nd1^{i}—Nd1—Rh1^{iv}	119.704 (1)	B1^{xii}—Rh1—Rh1^{xvi}	51.974 (1)
Nd1^{ii}—Nd1—Rh1^{iv}	60.296 (1)	B1^{xiii}—Rh1—Rh1^{xvi}	128.026 (2)
Rh1^{iii}—Nd1—Rh1^{iv}	180.0	B1^{xiv}—Rh1—Rh1^{xvi}	51.974 (1)
Nd1^{i}—Nd1—Rh1^{v}	60.296 (1)	Rh1^{xv}—Rh1—Rh1^{xvi}	180.0
Nd1^{ii}—Nd1—Rh1^{v}	119.704 (1)	B1^{xi}—Rh1—Rh1^{iii}	51.973 (1)
Rh1^{iii}—Nd1—Rh1^{v}	51.481 (1)	B1^{xii}—Rh1—Rh1^{iii}	128.027 (1)
Rh1^{iv}—Nd1—Rh1^{v}	128.519 (1)	B1^{xiii}—Rh1—Rh1^{iii}	51.973 (1)
Nd1^{i}—Nd1—Rh1^{vi}	119.704 (1)	B1^{xiv}—Rh1—Rh1^{iii}	128.027 (1)
Nd1^{ii}—Nd1—Rh1^{vi}	60.296 (1)	Rh1^{xv}—Rh1—Rh1^{iii}	60.0
Rh1^{iii}—Nd1—Rh1^{vi}	128.519 (1)	Rh1^{xvi}—Rh1—Rh1^{iii}	120.0
Rh1^{iv}—Nd1—Rh1^{vi}	51.481 (1)	B1^{xi}—Rh1—Rh1^{xvii}	128.027 (2)

Rh1^{v}—Nd1—Rh1^{vi}	180.0
Nd1^{i}—Nd1—Rh1	60.296 (1)
Nd1^{ii}—Nd1—Rh1	119.704 (1)
Rh1^{iii}—Nd1—Rh1	51.481 (1)
Rh1^{iv}—Nd1—Rh1	128.519 (1)
Rh1^{v}—Nd1—Rh1	97.568 (2)
Rh1^{vi}—Nd1—Rh1	82.432 (2)
Nd1^{i}—Nd1—Rh1^{vii}	119.704 (1)
Nd1^{ii}—Nd1—Rh1^{vii}	60.296 (1)
Rh1^{iii}—Nd1—Rh1^{vii}	128.519 (1)
Rh1^{iv}—Nd1—Rh1^{vii}	51.481 (1)
Rh1^{v}—Nd1—Rh1^{vii}	82.432 (2)
Rh1^{vi}—Nd1—Rh1^{vii}	97.568 (2)
Rh1—Nd1—Rh1^{vii}	180.0
Nd1^{i}—Nd1—Rh1^{viii}	60.296 (2)
Nd1^{ii}—Nd1—Rh1^{viii}	119.704 (2)
Rh1^{iii}—Nd1—Rh1^{viii}	120.592 (3)
Rh1^{iv}—Nd1—Rh1^{viii}	59.408 (3)
Rh1^{v}—Nd1—Rh1^{viii}	97.568 (2)
Rh1^{vi}—Nd1—Rh1^{viii}	82.432 (2)
Rh1—Nd1—Rh1^{viii}	97.568 (2)
Rh1^{vii}—Nd1—Rh1^{viii}	82.432 (2)
Nd1^{i}—Nd1—Rh1^{ix}	119.704 (2)
Nd1^{ii}—Nd1—Rh1^{ix}	60.296 (2)
Rh1^{iii}—Nd1—Rh1^{ix}	59.408 (3)
Rh1^{iv}—Nd1—Rh1^{ix}	120.592 (3)
Rh1^{v}—Nd1—Rh1^{ix}	82.432 (2)
Rh1^{vi}—Nd1—Rh1^{ix}	97.568 (2)
Rh1—Nd1—Rh1^{ix}	82.432 (2)
Rh1^{vii}—Nd1—Rh1^{ix}	97.568 (2)
Rh1^{viii}—Nd1—Rh1^{ix}	180.0
Nd1^{i}—Nd1—Rh1^{x}	60.296 (1)
Nd1^{ii}—Nd1—Rh1^{x}	119.704 (1)
Rh1^{iii}—Nd1—Rh1^{x}	97.568 (3)
Rh1^{iv}—Nd1—Rh1^{x}	82.432 (3)
Rh1^{v}—Nd1—Rh1^{x}	51.481 (1)
Rh1^{vi}—Nd1—Rh1^{x}	128.519 (1)
Rh1—Nd1—Rh1^{x}	120.592 (3)
Rh1^{vii}—Nd1—Rh1^{x}	59.408 (3)
Rh1^{viii}—Nd1—Rh1^{x}	51.481 (1)
Rh1^{ix}—Nd1—Rh1^{x}	128.519 (1)
Nd1^{i}—Nd1—Rh1^{ii}	119.704 (1)
Nd1^{ii}—Nd1—Rh1^{ii}	60.296 (1)
Rh1^{iii}—Nd1—Rh1^{ii}	82.432 (3)
Rh1^{iv}—Nd1—Rh1^{ii}	97.568 (3)
Rh1^{v}—Nd1—Rh1^{ii}	128.519 (1)
Rh1^{vi}—Nd1—Rh1^{ii}	51.481 (1)
Rh1—Nd1—Rh1^{ii}	59.408 (3)
B1^{xii}—Rh1—Rh1^{xvii}	51.973 (1)
B1^{xiii}—Rh1—Rh1^{xvii}	128.027 (1)
B1^{xiv}—Rh1—Rh1^{xvii}	51.973 (1)
Rh1^{xv}—Rh1—Rh1^{xvii}	120.0
Rh1^{xvi}—Rh1—Rh1^{xvii}	60.0
Rh1^{iii}—Rh1—Rh1^{xvii}	180.0
B1^{xi}—Rh1—Rh1^{i}	45.343 (2)
B1^{xii}—Rh1—Rh1^{i}	134.657 (1)
B1^{xiii}—Rh1—Rh1^{i}	134.657 (2)
B1^{xiv}—Rh1—Rh1^{i}	45.343 (2)
Rh1^{xv}—Rh1—Rh1^{i}	90.0
Rh1^{xvi}—Rh1—Rh1^{i}	90.0
Rh1^{iii}—Rh1—Rh1^{i}	90.0
Rh1^{xvii}—Rh1—Rh1^{i}	90.0
B1^{xi}—Rh1—Rh1^{ii}	134.657 (2)
B1^{xii}—Rh1—Rh1^{ii}	45.343 (2)
B1^{xiii}—Rh1—Rh1^{ii}	45.343 (2)
B1^{xiv}—Rh1—Rh1^{ii}	134.657 (2)
Rh1^{xv}—Rh1—Rh1^{ii}	90.0
Rh1^{xvi}—Rh1—Rh1^{ii}	90.0
Rh1^{iii}—Rh1—Rh1^{ii}	90.0
Rh1^{xvii}—Rh1—Rh1^{ii}	90.0
Rh1^{i}—Rh1—Rh1^{ii}	180.0
B1^{xi}—Rh1—Nd1	110.381 (2)
B1^{xii}—Rh1—Nd1	69.619 (2)
B1^{xiii}—Rh1—Nd1	69.617 (2)
B1^{xiv}—Rh1—Nd1	110.383 (2)
Rh1^{xv}—Rh1—Nd1	115.7
Rh1^{xvi}—Rh1—Nd1	64.3
Rh1^{iii}—Rh1—Nd1	64.259 (1)
Rh1^{xvii}—Rh1—Nd1	115.741 (1)
Rh1^{i}—Rh1—Nd1	119.704 (1)
Rh1^{ii}—Rh1—Nd1	60.296 (1)
B1^{xi}—Rh1—Nd1^{xviii}	69.619 (2)
B1^{xii}—Rh1—Nd1^{xviii}	110.381 (2)
B1^{xiii}—Rh1—Nd1^{xviii}	110.383 (2)
B1^{xiv}—Rh1—Nd1^{xviii}	69.617 (2)
Rh1^{xv}—Rh1—Nd1^{xviii}	64.3
Rh1^{xvi}—Rh1—Nd1^{xviii}	115.7
Rh1^{iii}—Rh1—Nd1^{xviii}	115.741 (1)
Rh1^{xvii}—Rh1—Nd1^{xviii}	64.259 (1)
Rh1^{i}—Rh1—Nd1^{xviii}	60.296 (1)
Rh1^{ii}—Rh1—Nd1^{xviii}	119.704 (1)
Nd1—Rh1—Nd1^{xviii}	180.0
Rh1^{xix}—B1—Rh1^{xx}	138.332 (1)
Rh1^{xix}—B1—Rh1^{v}	89.314 (4)
Rh1^{xx}—B1—Rh1^{v}	76.053 (3)
Rh1^{xix}—B1—Rh1^{xxi}	76.053 (3)

$Rh1^{vii}—Nd1—Rh1^{ii}$	120.592 (3)	$Rh1^{xx}—B1—Rh1^{xxi}$	89.314 (4)
$Rh1^{viii}—Nd1—Rh1^{ii}$	128.519 (1)	$Rh1^{v}—B1—Rh1^{xxi}$	138.332 (1)
$Rh1^{ix}—Nd1—Rh1^{ii}$	51.481 (1)	$Rh1^{xix}—B1—Rh1^{iii}$	138.332 (1)
$Rh1^{x}—Nd1—Rh1^{ii}$	180.0	$Rh1^{xx}—B1—Rh1^{iii}$	76.053 (2)
$B1^{xi}—Rh1—B1^{xii}$	180.0	$Rh1^{v}—B1—Rh1^{iii}$	76.053 (3)
$B1^{xi}—Rh1—B1^{xiii}$	89.314 (4)	$Rh1^{xxi}—B1—Rh1^{iii}$	138.332 (1)
$B1^{xii}—Rh1—B1^{xiii}$	90.686 (4)	$Rh1^{xix}—B1—Rh1^{ix}$	76.053 (3)
$B1^{xi}—Rh1—B1^{xiv}$	90.686 (4)	$Rh1^{xx}—B1—Rh1^{ix}$	138.332 (1)
$B1^{xii}—Rh1—B1^{xiv}$	89.314 (4)	$Rh1^{v}—B1—Rh1^{ix}$	138.332 (2)
$B1^{xiii}—Rh1—B1^{xiv}$	180.0	$Rh1^{xxi}—B1—Rh1^{ix}$	76.053 (3)
$B1^{xi}—Rh1—Rh1^{xv}$	51.974 (1)	$Rh1^{iii}—B1—Rh1^{ix}$	89.314 (4)
$B1^{xii}—Rh1—Rh1^{xv}$	128.026 (1)		

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*, *y*, *z*−1; (iii) −*x*+*y*+1, −*x*+1, *z*; (iv) −*x*+*y*, −*x*, *z*−1; (v) −*y*, *x*−*y*, *z*; (vi) −*y*, *x*−*y*−1, *z*−1; (vii) *x*−1, *y*, *z*−1; (viii) −*x*+*y*, −*x*, *z*; (ix) −*x*+*y*+1, −*x*+1, *z*−1; (x) *x*−1, *y*, *z*; (xi) −*x*+1, −*y*+1, −*z*+1; (xii) *x*, *y*−1, *z*; (xiii) −*x*+1, −*y*+1, −*z*; (xiv) *x*, *y*−1, *z*+1; (xv) −*y*+1, *x*−*y*, *z*; (xvi) −*y*, *x*−*y*−1, *z*; (xvii) −*x*+*y*+1, −*x*, *z*; (xviii) *x*+1, *y*, *z*+1; (xix) −*y*, *x*−*y*, *z*−1; (xx) *x*, *y*+1, *z*; (xxi) *x*, *y*+1, *z*−1.

Samarium trirhodium diboride (III)

Crystal data

$SmRh_3B_2$	D_x = 9.972 Mg m^{-3}
M_r = 480.70	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hexagonal, *P*6/*mmm*	Cell parameters from 649 reflections
a = 5.4438 (2) Å	θ = 4.3–40.1°
c = 3.11901 (12) Å	μ = 32.61 mm^{-1}
V = 80.05 (1) Å^3	*T* = 293 K
Z = 1	Block, metallic
F(000) = 207	0.06 × 0.05 × 0.02 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer	T_{min} = 0.324, T_{max} = 0.542
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source	696 measured reflections
Mirror monochromator	129 independent reflections
Detector resolution: 10.0000 pixels mm^{-1}	128 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.011
Absorption correction: numerical (CrysAlisPro; Rigaku OD, 2021)	θ_{max} = 40.1°, θ_{min} = 4.3°
	$h = -8 \rightarrow 9$
	$k = -7 \rightarrow 7$
	$l = -3 \rightarrow 5$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 0.0484P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	$(\Delta/\sigma)_{max} < 0.001$
$R[F^2 > 2\sigma(F^2)]$ = 0.012	$\Delta\rho_{max}$ = 1.76 e Å^{-3}
$wR(F^2)$ = 0.032	$\Delta\rho_{min}$ = −0.97 e Å^{-3}
S = 1.13	Extinction correction: SHELXL-2016/6 (Sheldrick 2016), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
129 reflections	Extinction coefficient: 0.034 (3)
9 parameters	
0 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Sm1	0.000000	0.000000	0.000000	0.00780 (10)
Rh1	0.500000	0.000000	0.500000	0.00739 (10)
B1	0.333333	0.666667	0.000000	0.0091 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.00841 (12)	0.00841 (12)	0.00658 (14)	0.00420 (6)	0.000	0.000
Rh1	0.00502 (11)	0.00389 (13)	0.01287 (14)	0.00194 (6)	0.000	0.000
B1	0.0085 (10)	0.0085 (10)	0.0102 (15)	0.0043 (5)	0.000	0.000

Geometric parameters (Å, º)

Sm1—Sm1^{i}	3.1190 (1)	Sm1—Rh1^{x}	3.1370 (1)
Sm1—Sm1^{ii}	3.1190 (1)	Rh1—B1^{xi}	2.2140 (1)
Sm1—Rh1^{iii}	3.1370 (1)	Rh1—B1^{xii}	2.2140 (1)
Sm1—Rh1^{iv}	3.1370 (1)	Rh1—B1^{xiii}	2.2140 (1)
Sm1—Rh1	3.1370 (1)	Rh1—B1^{xiv}	2.2140 (1)
Sm1—Rh1^{v}	3.1370 (1)	Rh1—Rh1^{xv}	2.7219 (1)
Sm1—Rh1^{vi}	3.1370 (1)	Rh1—Rh1^{xvi}	2.7219 (1)
Sm1—Rh1^{vii}	3.1370 (1)	Rh1—Rh1^{iii}	2.7219 (1)
Sm1—Rh1^{viii}	3.1370 (1)	Rh1—Rh1^{xvii}	2.7219 (1)
Sm1—Rh1^{ix}	3.1370 (1)	Rh1—Rh1^{i}	3.1190 (1)
Sm1—Rh1^{ii}	3.1370 (1)	Rh1—Rh1^{ii}	3.1190 (1)
Sm1^{i}—Sm1—Sm1^{ii}	180.0	B1^{xiii}—Rh1—Rh1^{xv}	52.069 (1)
Sm1^{i}—Sm1—Rh1^{iii}	60.189 (1)	B1^{xiv}—Rh1—Rh1^{xv}	127.931 (1)
Sm1^{ii}—Sm1—Rh1^{iii}	119.811 (1)	B1^{xi}—Rh1—Rh1^{xvi}	127.931 (1)
Sm1^{i}—Sm1—Rh1^{iv}	119.811 (1)	B1^{xii}—Rh1—Rh1^{xvi}	52.069 (1)
Sm1^{ii}—Sm1—Rh1^{iv}	60.189 (1)	B1^{xiii}—Rh1—Rh1^{xvi}	127.931 (1)
Rh1^{iii}—Sm1—Rh1^{iv}	180.0	B1^{xiv}—Rh1—Rh1^{xvi}	52.069 (1)
Sm1^{i}—Sm1—Rh1	60.189 (2)	Rh1^{xv}—Rh1—Rh1^{xvi}	180.0
Sm1^{ii}—Sm1—Rh1	119.811 (1)	B1^{xi}—Rh1—Rh1^{iii}	52.069 (1)
Rh1^{iii}—Sm1—Rh1	51.423 (1)	B1^{xii}—Rh1—Rh1^{iii}	127.931 (1)
Rh1^{iv}—Sm1—Rh1	128.6	B1^{xiii}—Rh1—Rh1^{iii}	52.069 (1)
Sm1^{i}—Sm1—Rh1^{v}	119.811 (1)	B1^{xiv}—Rh1—Rh1^{iii}	127.931 (1)
Sm1^{ii}—Sm1—Rh1^{v}	60.189 (2)	Rh1^{xv}—Rh1—Rh1^{iii}	60.0
Rh1^{iii}—Sm1—Rh1^{v}	128.6	Rh1^{xvi}—Rh1—Rh1^{iii}	120.0
Rh1^{iv}—Sm1—Rh1^{v}	51.423 (1)	B1^{xi}—Rh1—Rh1^{xvii}	127.931 (1)

Rh1—Sm1—Rh1^{v}	180.0	B1^{xii}—Rh1—Rh1^{xvii}	52.069 (1)
Sm1^{i}—Sm1—Rh1^{vi}	60.189 (2)	B1^{xiii}—Rh1—Rh1^{xvii}	127.931 (1)
Sm1^{ii}—Sm1—Rh1^{vi}	119.811 (1)	B1^{xiv}—Rh1—Rh1^{xvii}	52.069 (1)
Rh1^{iii}—Sm1—Rh1^{vi}	51.423 (1)	Rh1^{xv}—Rh1—Rh1^{xvii}	120.0
Rh1^{iv}—Sm1—Rh1^{vi}	128.577 (1)	Rh1^{xvi}—Rh1—Rh1^{xvii}	60.0
Rh1—Sm1—Rh1^{vi}	97.428 (2)	Rh1^{iii}—Rh1—Rh1^{xvii}	180.0
Rh1^{v}—Sm1—Rh1^{vi}	82.572 (2)	B1^{xi}—Rh1—Rh1^{i}	45.219 (1)
Sm1^{i}—Sm1—Rh1^{vii}	119.811 (1)	B1^{xii}—Rh1—Rh1^{i}	134.781 (2)
Sm1^{ii}—Sm1—Rh1^{vii}	60.189 (2)	B1^{xiii}—Rh1—Rh1^{i}	134.781 (1)
Rh1^{iii}—Sm1—Rh1^{vii}	128.577 (1)	B1^{xiv}—Rh1—Rh1^{i}	45.219 (1)
Rh1^{iv}—Sm1—Rh1^{vii}	51.423 (1)	Rh1^{xv}—Rh1—Rh1^{i}	90.0
Rh1—Sm1—Rh1^{vii}	82.572 (2)	Rh1^{xvi}—Rh1—Rh1^{i}	90.0
Rh1^{v}—Sm1—Rh1^{vii}	97.428 (2)	Rh1^{iii}—Rh1—Rh1^{i}	90.0
Rh1^{vi}—Sm1—Rh1^{vii}	180.0	Rh1^{xvii}—Rh1—Rh1^{i}	90.0
Sm1^{i}—Sm1—Rh1^{viii}	60.189 (1)	B1^{xi}—Rh1—Rh1^{ii}	134.781 (2)
Sm1^{ii}—Sm1—Rh1^{viii}	119.811 (1)	B1^{xii}—Rh1—Rh1^{ii}	45.219 (2)
Rh1^{iii}—Sm1—Rh1^{viii}	120.379 (3)	B1^{xiii}—Rh1—Rh1^{ii}	45.219 (1)
Rh1^{iv}—Sm1—Rh1^{viii}	59.621 (3)	B1^{xiv}—Rh1—Rh1^{ii}	134.781 (1)
Rh1—Sm1—Rh1^{viii}	97.428 (2)	Rh1^{xv}—Rh1—Rh1^{ii}	90.0
Rh1^{v}—Sm1—Rh1^{viii}	82.572 (2)	Rh1^{xvi}—Rh1—Rh1^{ii}	90.0
Rh1^{vi}—Sm1—Rh1^{viii}	97.428 (1)	Rh1^{iii}—Rh1—Rh1^{ii}	90.0
Rh1^{vii}—Sm1—Rh1^{viii}	82.572 (1)	Rh1^{xvii}—Rh1—Rh1^{ii}	90.0
Sm1^{i}—Sm1—Rh1^{ix}	119.811 (1)	Rh1^{i}—Rh1—Rh1^{ii}	180.0
Sm1^{ii}—Sm1—Rh1^{ix}	60.189 (1)	B1^{xi}—Rh1—Sm1	110.498 (2)
Rh1^{iii}—Sm1—Rh1^{ix}	59.621 (3)	B1^{xii}—Rh1—Sm1	69.502 (1)
Rh1^{iv}—Sm1—Rh1^{ix}	120.379 (3)	B1^{xiii}—Rh1—Sm1	69.501 (1)
Rh1—Sm1—Rh1^{ix}	82.572 (2)	B1^{xiv}—Rh1—Sm1	110.499 (1)
Rh1^{v}—Sm1—Rh1^{ix}	97.428 (2)	Rh1^{xv}—Rh1—Sm1	115.711 (1)
Rh1^{vi}—Sm1—Rh1^{ix}	82.572 (1)	Rh1^{xvi}—Rh1—Sm1	64.3
Rh1^{vii}—Sm1—Rh1^{ix}	97.428 (1)	Rh1^{iii}—Rh1—Sm1	64.289 (1)
Rh1^{viii}—Sm1—Rh1^{ix}	180.0	Rh1^{xvii}—Rh1—Sm1	115.7
Sm1^{i}—Sm1—Rh1^{ii}	119.811 (1)	Rh1^{i}—Rh1—Sm1	119.811 (2)
Sm1^{ii}—Sm1—Rh1^{ii}	60.189 (1)	Rh1^{ii}—Rh1—Sm1	60.189 (2)
Rh1^{iii}—Sm1—Rh1^{ii}	82.572 (2)	B1^{xi}—Rh1—Sm1^{xviii}	69.502 (2)
Rh1^{iv}—Sm1—Rh1^{ii}	97.428 (2)	B1^{xii}—Rh1—Sm1^{xviii}	110.498 (1)
Rh1—Sm1—Rh1^{ii}	59.621 (3)	B1^{xiii}—Rh1—Sm1^{xviii}	110.499 (1)
Rh1^{v}—Sm1—Rh1^{ii}	120.379 (4)	B1^{xiv}—Rh1—Sm1^{xviii}	69.501 (1)
Rh1^{vi}—Sm1—Rh1^{ii}	128.577 (1)	Rh1^{xv}—Rh1—Sm1^{xviii}	64.3
Rh1^{vii}—Sm1—Rh1^{ii}	51.423 (1)	Rh1^{xvi}—Rh1—Sm1^{xviii}	115.7
Rh1^{viii}—Sm1—Rh1^{ii}	128.577 (1)	Rh1^{iii}—Rh1—Sm1^{xviii}	115.7
Rh1^{ix}—Sm1—Rh1^{ii}	51.423 (1)	Rh1^{xvii}—Rh1—Sm1^{xviii}	64.3
Sm1^{i}—Sm1—Rh1^{x}	60.189 (1)	Rh1^{i}—Rh1—Sm1^{xviii}	60.189 (1)
Sm1^{ii}—Sm1—Rh1^{x}	119.811 (1)	Rh1^{ii}—Rh1—Sm1^{xviii}	119.811 (1)
Rh1^{iii}—Sm1—Rh1^{x}	97.428 (2)	Sm1—Rh1—Sm1^{xviii}	180.0
Rh1^{iv}—Sm1—Rh1^{x}	82.572 (2)	Rh1^{xix}—B1—Rh1^{xx}	138.425 (1)
Rh1—Sm1—Rh1^{x}	120.379 (4)	Rh1^{xix}—B1—Rh1^{xxi}	75.862 (3)
Rh1^{v}—Sm1—Rh1^{x}	59.621 (3)	Rh1^{xx}—B1—Rh1^{xxi}	89.562 (4)
Rh1^{vi}—Sm1—Rh1^{x}	51.423 (1)	Rh1^{xix}—B1—Rh1^{vi}	89.562 (4)

Rh1^{vii}—Sm1—Rh1^{x}	128.577 (1)	Rh1^{xx}—B1—Rh1^{vi}	75.862 (3)
Rh1^{viii}—Sm1—Rh1^{x}	51.423 (1)	Rh1^{xxi}—B1—Rh1^{vi}	138.425 (1)
Rh1^{ix}—Sm1—Rh1^{x}	128.577 (1)	Rh1^{xix}—B1—Rh1^{iii}	138.425 (1)
Rh1^{ii}—Sm1—Rh1^{x}	180.0	Rh1^{xx}—B1—Rh1^{iii}	75.862 (3)
B1^{xi}—Rh1—B1^{xii}	180.0	Rh1^{xxi}—B1—Rh1^{iii}	138.425 (1)
B1^{xi}—Rh1—B1^{xiii}	89.561 (4)	Rh1^{vi}—B1—Rh1^{iii}	75.862 (3)
B1^{xii}—Rh1—B1^{xiii}	90.439 (4)	Rh1^{xix}—B1—Rh1^{ix}	75.862 (2)
B1^{xi}—Rh1—B1^{xiv}	90.439 (4)	Rh1^{xx}—B1—Rh1^{ix}	138.425 (1)
B1^{xii}—Rh1—B1^{xiv}	89.561 (4)	Rh1^{xxi}—B1—Rh1^{ix}	75.862 (3)
B1^{xiii}—Rh1—B1^{xiv}	180.0	Rh1^{vi}—B1—Rh1^{ix}	138.425 (1)
B1^{xi}—Rh1—Rh1^{xv}	52.069 (1)	Rh1^{iii}—B1—Rh1^{ix}	89.562 (4)
B1^{xii}—Rh1—Rh1^{xv}	127.931 (1)		

Symmetry codes: (i) $x, y, z+1$; (ii) $x, y, z-1$; (iii) $-x+y+1, -x+1, z$; (iv) $-x+y, -x, z-1$; (v) $x-1, y, z-1$; (vi) $-y, x-y, z$; (vii) $-y, x-y-1, z-1$; (viii) $-x+y, -x, z$; (ix) $-x+y+1, -x+1, z-1$; (x) $x-1, y, z$; (xi) $-x+1, -y+1, -z+1$; (xii) $x, y-1, z$; (xiii) $-x+1, -y+1, -z$; (xiv) $x, y-1, z+1$; (xv) $-y+1, x-y, z$; (xvi) $-y, x-y-1, z$; (xvii) $-x+y+1, -x, z$; (xviii) $x+1, y, z+1$; (xix) $-y, x-y, z-1$; (xx) $x, y+1, z$; (xxi) $x, y+1, z-1$.