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

Makoto Tokuda,* Kunio Yubuta, Toetsu Shishido and Kazumasa Sugiyama

The crystal structures of the rare-earth (\( RE \)) trirhodium diborides praseodymium trirhodium diboride, \( \text{PrRh}_3\text{B}_2 \), neodymium trirhodium diboride, \( \text{NdRh}_3\text{B}_2 \), and samarium trirhodium diboride, \( \text{SmRh}_3\text{B}_2 \), were refined on the basis of single-crystal X-ray diffraction data. The crystal chemistry of \( RERh_3B_2 \) (\( RE: \text{Pr, Nd, and Sm} \)) 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 \( \text{CeRh}_3\text{B}_2 \); \( RE \), Rh and B sites are situated on special positions with site symmetry 6/mmm (Wyckoff position 1a), mmm (3g) and 6m2 (2c), respectively. In comparison with the previous powder X-ray study of hexagonal \( \text{CeRh}_3\text{B}_2 \), 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$_3$B$_2$-type \( RERh_3B_2 \) (\( RE = \text{rare-earth element} \)) 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 \( \text{CeRh}_3\text{B}_2 \) by using single-crystal XRD data and discussed the characteristics of the anisotropic atomic displacement parameters (ADPs) of atoms in \( \text{CeRh}_3\text{B}_2 \) in relation to the structure. We report here the results of structural refinements using single crystals of \( RERh_3B_2 \) (\( RE = \text{Pr, Nd, and Sm} \)) grown by the arc-melting method.

2. Structural commentary

The crystal structures of hexagonal \( RERh_3B_2 \) (\( RE: \text{La–Gd} \)) compounds are isotypic with \( \text{CeCo}_3\text{B}_2 \) and crystallize in space-group type \( \text{P6}_3/mmm \) (Kuz’ma et al., 1969). The \( \text{CeCo}_3\text{B}_2 \) type of structure is ordered and can be derived from the \( \text{CaCu}_3 \) 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 \( \text{[BRh}_6\text{]} \)
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 $RERh_{3}B_{2}$ type of structure can also be described as being built up of kagomé layers of Rh atoms stacked along the $c$ axis with an $a\alpha$ 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 $RERh_{3}B_{2}$ ($RE$ = 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 $RERh_{3}B_{2}$ compounds change anisotropically, suggesting that the unit-cell changes elastically in response to the substitution of elements of different sizes at the $RE$ site.

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

Table 1

|        | $PrRh_{3}B_{2}$ | $NdRh_{3}B_{2}$ | $SmRh_{3}B_{2}$ |
|--------|-----------------|-----------------|-----------------|
| $RE$–$RE$ $x2$ | 3.1084 (1)       | 3.1107 (1)       | 3.1190 (1)       |
| $RE$–$RE$ $x6$ | 5.4676 (4)       | 5.4527 (3)       | 5.4438 (3)       |
| $RE$–Rh $x12$ | 3.1447 (1)       | 3.1388 (1)       | 3.1370 (1)       |
| $RE$–B $x6$   | 3.1557 (2)       | 3.1481 (1)       | 3.1430 (1)       |
| B–Rh $x6$    | 2.2151 (1)       | 2.2129 (1)       | 2.2140 (1)       |
| B–B $x3$     | 3.1084 (1)       | 3.1107 (1)       | 3.1190 (1)       |
| Rh–Rh $x4$   | 2.7338 (2)       | 2.7264 (1)       | 2.7219 (1)       |
| Rh–Rh $x2$   | 3.1084 (1)       | 3.1107 (1)       | 3.1190 (1)       |

Figure 1
Structure of $RERh_{3}B_{2}$ 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.

Figure 2
Unit-cell parameters $a$ (circles), $c$ (squares) and unit-cell volume (triangles) of $RERh_{3}B_{2}$ compounds. Closed and open marks refer to this study and previous work (Malik et al., 1983), respectively.
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 $\text{RE} \text{Rh}_3\text{B}_2$ compounds (Yamada et al., 2004; Obiraki et al., 2006). The ADPs of $\text{RE}$ atoms are described as displacement ellipsoids suppressed in the $c$ axis ($U_{11} < U_{33}$). The feature of displacement ellipsoids of Rh and $\text{RE}$ atoms is attributed to the unusually short $\text{RE}$—$\text{RE}$ 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 $\text{RE}$—$\text{RE}$ interatomic distance is a common feature of the CeCo$_3$B$_2$ type of structure.

3. Synthesis and crystallization

$\text{RE} \text{Rh}_3\text{B}_2$ ($\text{RE} = \text{Pr}, \text{Nd}, \text{and Sm}$) single crystals were grown using the arc-melting method. The starting materials used were $\text{RE}$ elements (99.9%), along with Rh (99.95%), and B (99.5%). They were weighed at an atomic ratio of $(\text{RE} + 3\text{Rh} + 2\text{B})$, 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 $\text{RE} \text{Rh}_3\text{B}_2$, and the atomic ratio Rh/$\text{RE}$ 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 $P6_3/mmm$, as reported by Ku et al. (1980). Based on structural reports of $\text{La}_{1-x}\text{Rh}_3\text{B}_2$ and $\text{Nd}_{1-x}\text{Rh}_3\text{B}_2$, we determined whether Rh substitution and vacancies at the $\text{RE}$ site were possible; however, the results were negative. Therefore, we concluded that the $\text{RE}$ sites were completely occupied by $\text{RE}$ 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 $\text{RE}$ heavy elements are censoring effects caused by the finite Fourier series.
Table 3
Experimental details.

| Crystal data | PrRh₃B₂ | NdRh₃B₂ | SmRh₃B₂ |
|--------------|---------|---------|---------|
| M₀           | 471.26  | 474.59  | 480.70  |
| Crystal system, space group | Hexagonal, P6/mmm | Hexagonal, P6/mmm | Hexagonal, P6/mmm |
| a, c (Å)     | 5.4676 (3), 3.10837 (16) | 5.4527 (2), 3.11066 (13) | 5.4438 (2), 3.11901 (12) |
| V (Å³)       | 80.47 (1) | 80.10 (1) | 80.05 (1) |
| Z             | 1       | 1       | 1       |
| Radiation type | Mo Kα   | Mo Kα   | Mo Kα   |
| μ (mm⁻¹)     | 29.45   | 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 Numerical (CrysAlis PRO; Rigaku OD, 2021) | XtaLAB Synergy, Dualflex, HyPix Numerical (CrysAlis PRO; Rigaku OD, 2021) | XtaLAB Synergy, Dualflex, HyPix Numerical (CrysAlis PRO; Rigaku OD, 2021) |
|----------------|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------|
| Tₘin, Tₘax   | 0.0423, 0.601                                                                   | 0.424, 0.611                                                                   | 0.324, 0.542                                                                   |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 733, 131, 126                                                                   | 827, 131, 130                                                                   | 696, 129, 128                                                                   |
| Rint         | 0.017                                                                          | 0.010                                                                          | 0.011                                                                          |
| (sin θ/λ)ₘax (Å⁻¹) | 0.909                                                                      | 0.908                                                                          | 0.907                                                                          |

Refinement

| R[F² > 2σ(F²)], wR(F²), 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                 |
| Δρₘax, Δρₘin (e Å⁻³)       | 1.80, —1.18       | 0.97, —2.46       | 1.76, —0.97       |

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

Funding information

We gratefully acknowledge the support from JSPS KAKENHI grant Nos. JP19K05643 (KY) and JP20H05258 (KY).

References

Daane, A. H., Rundle, R. E., Smith, H. G. & Spedding, F. H. (1954). Acta Cryst. 7, 532–535.
Higashi, I., Kasaya, M., Okabe, A. & Kasuya, T. (1987). J. Solid State Chem. 69, 376–379.
Higashi, I., Shishido, T., Takei, H. & Kobayashi, T. (1988). J. Less-Common Chem. 139, 211–220.
Hu, H. C., Ma, L. J., Tai, M. F., Wang, Y. & Horng, H. E. (1985). J. Less-Common Met. 109, 219–228.
Hu, H. C. & Meisner, G. P. (1981). J. Less-Common Met. 78, 99–107.
Hu, H. C., Meisner, G. P., Acker, F. & Johnston, D. C. (1980). Solid State Commun. 35, 91–96.
Kuz'ma, Y. B., Krypyakeych, P. I. & Bilonizhko, N. S. (1969). Dopov. Akad. Nauk Ukr. RSR Ser. A. pp. 939–941.
Malik, S. K., Vijayaraghavan, R., Wallace, W. E. & Dhar, S. K. (1983). J. Magn. Magn. Mater. 37, 303–308.
Momma, K. & Izumi, F. (2011). J. Appl. Cryst. 44, 1272–1276.
Obiraki, Y., Nakashima, H., Galatanu, A., Matsuda, T. D., Haga, Y., Takeuchi, T., Sugiyama, K., Kindo, K., Hagiwara, M., Settai, R., Harima, H. & Onuki, Y. (2006). J. Phys. Soc. Jpn, 75, 064702.
Ohtani, T., Chevalier, B., Lejay, P., Etourneau, J., Vlasse, M. & Hagenmuller, P. (1983). J. Appl. Phys. 54, 5928–5934.
Rigaku OD (2021). CrysAlis PRO, Rigaku Corporation, Oxford, England.
Sheldrick, G. M. (2015a). Acta Cryst. A71, 3–8.
Sheldrick, G. M. (2015b). Acta Cryst. C71, 3–8.
Spedding, F. H., Daane, A. H. & Herrmann, K. W. (1956). Acta Cryst. 9, 559–563.
Vlasse, M., Ohtani, T., Chevalier, B. & Etourneau, J. (1983). J. Solid State Chem. 48, 188–192.
Westrip, S. P. (2010). J. Appl. Cryst. 43, 920–925.
Yamada, M., Obiraki, Y., Okubo, T., Shiromoto, T., Kida, Y., Shiomoto, M., Kohara, H., Yamamoto, T., Honda, D., Galatanu, A., Haga, Y., Takeuchi, T., Sugiyama, K., Settai, R., Kindo, K., Dhar, S. K., Harima, H. & Onuki, Y. (2004). J. Phys. Soc. Jpn, 73, 2266–2275.
Zachariasen, W. H. (1973). J. Inorg. Nucl. Chem. 35, 3487–3497.
Redetermination of the crystal structures of rare-earth trirhodium diboride \( RERh_3B_2 \) (\( RE = \text{Pr, Nd and Sm} \)) from single-crystal X-ray data

Makoto Tokuda, Kunio Yubuta, Toetsu Shishido and Kazumasa Sugiyama

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

Praseodymium trirhodium diboride (I)

\textit{Crystal data}

PrRh\(_3\)B\(_2\)

\( M_r = 471.26 \)

Hexagonal, \( P6/\overline{mmm} \)

\( a = 5.4676 \) (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, \( \lambda = 0.71073 \) Å

Cell parameters from 623 reflections

\( \theta = 4.3-39.9^\circ \)

\( \mu = 29.43 \) mm\(^{-1}\)

\( T = 293 \) K

Block, metallic

0.05 \times 0.03 \times 0.03 \) mm

\textit{Data collection}

XtaLAB Synergy, Dualflex, HyPix

\( T_{\min} = 0.423, T_{\max} = 0.601 \)

733 measured reflections

131 independent reflections

126 reflections with \( I > 2\sigma(I) \)

\( R_{\text{int}} = 0.017 \)

\( \theta_{\text{max}} = 40.3^\circ, \theta_{\text{min}} = 4.3^\circ \)

\( h = -9 \rightarrow 7 \)

\( k = -9 \rightarrow 9 \)

\( l = -3 \rightarrow 5 \)

\textit{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 \( P = (F_o^2 + 2F_c^2)/3 \)

\( (\Delta\sigma)_{\text{max}} < 0.001 \)

\( \Delta \rho_{\text{max}} = 1.80 \) e Å\(^{-3}\)

\( \Delta \rho_{\text{min}} = -1.18 \) 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)**

| Atom | x       | y       | z       | Uiso* / Ueq  |
|------|---------|---------|---------|--------------|
| Pr1  | 0.00000 | 0.00000 | 0.00000 | 0.00835 (14) |
| Rh1  | 0.50000 | 0.00000 | 0.50000 | 0.00653 (13) |
| B1   | 0.33333 | 0.66667 | 0.00000 | 0.0093 (10)  |

**Atomic displacement parameters (Å²)**

| Atom | U₁₁ | U₂₂ | U₃₃ | U₁₂ | U₁₃ | U₂₃ |
|------|-----|-----|-----|-----|-----|-----|
| 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, °)**

| Bond/Angle | Distance/Value |
|------------|----------------|
| Pr1—Pr1   | 3.1084 (2)     |
| Pr1—Pr1   | 3.1084 (2)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Rh1   | 3.1447 (1)     |
| Pr1—Pr1   | 180.0          |
| Pr1—Pr1   | 60.381 (1)     |
| Pr1—Pr1   | 119.619 (1)    |
| Pr1—Pr1   | 119.619 (1)    |
| Pr1—Pr1   | 60.381 (1)     |
| Pr1—Pr1   | 180.0          |
| Pr1—Pr1   | 60.381 (2)     |
| Pr1—Pr1   | 119.619 (2)    |
| Pr1—Pr1   | 51.528 (1)     |
| Pr1—Pr1   | 51.528 (1)     |
| Pr1—Pr1   | 60.381 (2)     |
| Pr1—Pr1   | 128.472 (1)    |
| Pr1—Pr1   | 119.619 (2)    |
| Pr1—Pr1   | 60.381 (2)     |
| Pr1—Pr1   | 128.472 (1)    |
| Pr1—Pr1   | 51.528 (1)     |
Rh1—Pr1—Rh1'  180.0  
Pr1—Pr1—Rh1 vi  60.381 (2)  
Pr1—Pr1—Rh1 vii  119.619 (2)  
Rh1—Pr1—Rh1 vi  51.528 (1)  
Rh1 vi—Pr1—Rh1 vi  128.472 (1)  
Rh1—Pr1—Rh1 vii  97.678 (2)  
Rh1 vi—Pr1—Rh1 vii  82.322 (2)  
Pr1—Pr1—Rh1 vii  119.619 (2)  
Pr1—Pr1—Rh1 viii  60.381 (2)  
Rh1—Pr1—Rh1 viii  128.472 (1)  
Rh1—Pr1—Rh1 viii  51.528 (1)  
Rh1—Pr1—Rh1 viii  120.763 (4)  
Rh1—Pr1—Rh1 viii  82.322 (3)  
Rh1 vi—Pr1—Rh1 viii  97.678 (2)  
Rh1 vi—Pr1—Rh1 viii  180.0  
Pr1—Pr1—Rh1 viii  60.381 (2)  
Pr1—Pr1—Rh1 viiii  119.619 (2)  
Rh1—Pr1—Rh1 viiii  59.238 (4)  
Rh1—Pr1—Rh1 viiii  120.763 (4)  
Rh1—Pr1—Rh1 viiii  82.322 (3)  
Rh1 vi—Pr1—Rh1 viiii  97.678 (3)  
Rh1 vi—Pr1—Rh1 viiii  82.322 (3)  
Rh1 vi—Pr1—Rh1 viiii  97.678 (3)  
Rh1 vi—Pr1—Rh1 viiii  180.0  
Pr1—Pr1—Rh1 viii  119.619 (2)  
Pr1—Pr1—Rh1 ix  60.381 (2)  
Rh1—Pr1—Rh1 ix  59.238 (4)  
Rh1—Pr1—Rh1 ix  120.763 (4)  
Rh1—Pr1—Rh1 ix  82.322 (3)  
Rh1—Pr1—Rh1 ix  97.678 (3)  
Rh1 vi—Pr1—Rh1 ix  82.322 (3)  
Rh1 vi—Pr1—Rh1 ix  97.678 (3)  
Rh1 vi—Pr1—Rh1 ix  180.0  
Pr1—Pr1—Rh1 ix  119.619 (2)  
Pr1—Pr1—Rh1 ix  60.381 (2)  
Rh1—Pr1—Rh1 iy  82.322 (3)  
Rh1—Pr1—Rh1 iy  97.678 (3)  
Rh1 i—Pr1—Rh1 iy  59.238 (4)  
Rh1 i—Pr1—Rh1 iy  120.762 (4)  
Rh1 vi—Pr1—Rh1 iy  128.472 (1)  
Rh1 vi—Pr1—Rh1 iy  128.472 (1)  
Rh1 vi—Pr1—Rh1 iy  51.528 (1)  
Pr1—Pr1—Rh1 i  60.381 (2)  
Pr1—Pr1—Rh1 i  119.619 (2)  
Rh1—Pr1—Rh1 i  51.528 (1)  
Rh1—Pr1—Rh1 i  128.472 (1)  
Rh1—Pr1—Rh1 i  82.322 (3)  
Rh1 vi—Pr1—Rh1 i  120.762 (4)  
Rh1 vi—Pr1—Rh1 i  59.238 (4)  
Rh1 vi—Pr1—Rh1 i  51.528 (1)
| Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|-------------|--------------|-------------|
| Rh1vi—Pr1—Rh1x | 128.472 (1) | Rh1vi—B1—Rh1xi | 89.116 (4) |
| Rh1vi—Pr1—Rh1x | 51.528 (1)  | Rh1vi—B1—Rh1xi | 138.257 (2) |
| Rh1ui—Pr1—Rh1x | 128.472 (1) | Rh1ix—B1—Rh1xi | 76.206 (4) |
| Rh1ii—Pr1—Rh1x | 180.0       | Rh1ix—B1—Rh1xi | 138.257 (2) |
| Rh1ui—Pr1—Rh1x | 180.0       | Rh1xx—B1—Rh1xi | 76.206 (4) |
| B1xi—Rh1—B1xii | 89.116 (4)  | B1xii—Rh1—B1xi | 138.257 (2) |
| B1xii—Rh1—B1xiii | 90.884 (4) | B1xi—Rh1—B1xii | 180.0       |
| B1xiii—Rh1—B1xiv | 90.884 (4) | B1xi—Rh1—B1xiii | 90.884 (4) |
| B1xiv—Rh1—B1xv  | 90.884 (4)  | B1xi—Rh1—B1xv  | 90.884 (4)  |
| B1xvi—Rh1—B1xv  | 90.884 (4)  | B1xi—Rh1—B1xv  | 90.884 (4)  |
| B1xv—B1—Rh1x    | 90.884 (4)  | B1xi—Rh1—B1xv  | 90.884 (4)  |
| B1xii—Rh1—B1xiii | 90.884 (4) | B1xi—Rh1—B1xv  | 90.884 (4)  |
| B1xiii—Rh1—B1xv  | 90.884 (4)  | B1xi—Rh1—B1xv  | 90.884 (4)  |
| B1x—B1—Rh1x     | 90.884 (4)  | B1xi—Rh1—B1xv  | 90.884 (4)  |
| B1xiii—Rh1—B1xv  | 90.884 (4)  | B1xi—Rh1—B1xv  | 90.884 (4)  |

Symmetry codes: (i) x, y, z+1; (ii) x, y, z−1; (iii) −x+y1, −x+z−1; (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+y1, −x−1, z−1; (x) x−1, y, z; (xi) x−y, x−y, z; (xii) −x+y1, −x−1, z−1; (xiii) −x+y, −x−1, z; (xiv) x, y−1, z−1; (xv) −y, x−y, z; (xvi) −y, x−y−1, z; (xvii) −x+y1, −x, z; (xviii) x+y1, 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

NdRh3B2

$M_r = 474.59$

Hexagonal, $P6_3/mmc$

$a = 5.4527 (2) \, \text{Å}$

$c = 3.11066 (13) \, \text{Å}$

$V = 80.10 (1) \, \text{Å}^3$

$Z = 1$

$F(000) = 205$

$D_x = 9.839 \, \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \, \text{Å}$

Cell parameters from 729 reflections

$\theta = 4.3-40.7^\circ$

$\mu = 30.57 \, \text{mm}^{-1}$

$T = 293 \, \text{K}$

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$^{-1}$

$\omega$ scans

Absorption correction: numerical
(CrystalClear; Rigaku OD, 2021)

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 $P = (F_o^2 + 2F_c^2)/3$

$\Delta\sigma_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.97 \, \text{e Å}^{-3}$

$\Delta\rho_{\text{min}} = -2.46 \, \text{e Å}^{-3}$

Acta Cryst. (2022). E78, 76-79
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      | Uiso* / Ueq |
|------|--------|--------|--------|-------------|
| 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)

|      | U₁₁   | U₂₂   | U₃₃   | U₁₂   | U₁₃   | U₂₃   |
|------|-------|-------|-------|-------|-------|-------|
| Nd1  | 0.00896 (10) | 0.00896 (10) | 0.00662 (12) | 0.00448 (5) | 0.000000 | 0.000000 |
| Rh1  | 0.00492 (9)  | 0.00390 (11)  | 0.01104 (12)  | 0.00195 (5)  | 0.000000 | 0.000000 |
| B1   | 0.01000 (9)   | 0.01000 (9)   | 0.00790 (12)   | 0.00500 (4)   | 0.000000 | 0.000000 |

Geometric parameters (Å, °)

|              | Nd1—Nd1¹  | Nd1—Rh1¹¹ | Nd1—Rh1¹² |
|--------------|------------|------------|------------|
| Nd1—Nd1¹    | 3.1107 (1) | 3.1388 (1) | 3.1388 (1) |
| Nd1—Nd1¹¹   | 3.1107 (1) | 3.1107 (1) | 2.2129 (1) |
| Nd1—Rh1¹¹   | 3.1388 (1) | 3.1388 (1) | 2.2129 (1) |
| Nd1—Rh1¹²   | 3.1388 (1) | 3.1388 (1) | 2.2129 (1) |

|              | Nd1—Nd1—Nd1¹¹  | Nd1—Rh1—B1¹    | Nd1—Rh1—B1¹² |
|--------------|-----------------|----------------|--------------|
| Nd1—Nd1—Nd1¹¹| 180.0           | B1¹—Rh1—Rh1¹²  | 51.974 (1)   |
| Nd1—Nd1—Rh1¹²| 60.296 (1)      | B1¹—Rh1—Rh1¹²  | 128.026 (1)  |

Acta Cryst. (2022), E78, 76-79
| Bond                        | Angle (°) | Bond                        | Angle (°) |
|---------------------------|-----------|---------------------------|-----------|
| Rh1v—Nd1—Rh1vi            | 180.0     | B1ii—Rh1—Rh1vii           | 51.973    |
| Nd1i—Nd1—Rh1              | 60.296    | B1ii—Rh1—Rh1vi            | 128.027   |
| Nd1ii—Nd1—Rh1             | 119.704   | B1iv—Rh1—Rh1vii           | 51.973    |
| Rh1vii—Nd1—Rh1            | 51.481    | Rh1vii—Rh1—Rh1vii         | 120.0     |
| Rh1vi—Nd1—Rh1             | 128.519   | Rh1vi—Rh1—Rh1vii          | 60.0      |
| Rh1vi—Nd1—Rh1             | 97.568    | Rh1viii—Rh1—Rh1vii        | 180.0     |
| Rh1vi—Nd1—Rh1             | 51.481    | B1i—Rh1—Rh1i              | 45.343    |
| Rh1vii—Nd1—Rh1            | 82.432    | B1ii—Rh1—Rh1i             | 134.657   |
| Nd1i—Nd1—Rh1vii           | 60.296    | B1iv—Rh1—Rh1i             | 45.343    |
| Rh1viii—Nd1—Rh1vii        | 180.0     | Rh1viii—Rh1—Rh1vii        | 134.657   |
| Rh1vii—Nd1—Rh1vii         | 60.296    | Rh1vi—Rh1—Rh1viii         | 90.0      |
| Rh1v—Nd1—Rh1vii           | 128.519   | Rh1vii—Rh1—Rh1vii         | 90.0      |
| Rh1v—Nd1—Rh1vii           | 97.568    | Rh1viii—Rh1—Rh1vii        | 90.0      |
| Rh1—Nd1—Rh1vii            | 180.0     | Rh1viii—Rh1—Rh1vii        | 90.0      |
| Nd1i—Nd1—Rh1viii          | 60.296    | B1i—Rh1—Rh1i              | 134.657   |
| Nd1ii—Nd1—Rh1viii         | 119.704   | B1ii—Rh1—Rh1i             | 45.343    |
| Rh1v—Nd1—Rh1viii          | 51.481    | B1iv—Rh1—Rh1i             | 45.343    |
| Rh1vi—Nd1—Rh1viii         | 82.432    | Rh1viii—Rh1—Rh1vii        | 134.657   |
| Rh1—Nd1—Rh1vii            | 97.568    | Rh1vi—Rh1—Rh1viii         | 90.0      |
| Rh1—Nd1—Rh1vii            | 60.296    | Rh1vii—Rh1—Rh1viii        | 90.0      |
| Nd1i—Nd1—Rh1x             | 119.704   | Rh1vi—Rh1—Rh1vii          | 90.0      |
| Nd1ii—Nd1—Rh1x            | 60.296    | Rh1vii—Rh1—Rh1vii         | 180.0     |
| Rh1v—Nd1—Rh1x             | 59.408    | B1i—Rh1—Rh1i              | 134.657   |
| Rh1vi—Nd1—Rh1x            | 120.592   | B1ii—Rh1—Rh1i             | 69.619    |
| Rh1—Nd1—Rh1x              | 82.432    | B1iv—Rh1—Rh1i             | 69.617    |
| Rh1—Nd1—Rh1x              | 97.568    | Rh1viii—Rh1—Rh1vii        | 110.383   |
| Rh1—Nd1—Rh1x              | 82.432    | Rh1vii—Rh1—Rh1vii         | 115.7     |
| Nd1i—Nd1—Rh1x             | 119.704   | Rh1vi—Rh1—Rh1vii          | 64.3      |
| Nd1ii—Nd1—Rh1x            | 60.296    | Rh1vii—Rh1—Nd1            | 64.259    |
| Rh1v—Nd1—Rh1x             | 59.408    | Rh1viii—Rh1—Nd1           | 115.741   |
| Rh1vi—Nd1—Rh1x            | 120.592   | Rh1—Rh1—Nd1               | 119.704   |
| Rh1—Nd1—Rh1x              | 82.432    | Rh1—Nd1—Rh1x              | 60.296    |
| Rh1—Nd1—Rh1x              | 97.568    | B1i—Rh1—Nd1               | 69.619    |
| Nd1i—Nd1—Rh1              | 60.296    | B1ii—Rh1—Nd1              | 110.381   |
| Nd1ii—Nd1—Rh1             | 119.704   | B1iv—Rh1—Nd1              | 69.617    |
| Rh1—Nd1—Rh1              | 59.408    | Rh1viii—Rh1—Nd1           | 110.383   |
| Rh1—Nd1—Rh1              | 97.568    | Rh1vii—Rh1—Nd1            | 69.617    |
| Nd1i—Nd1—Rh1              | 120.592   | Rh1v—Rh1—Nd1viii          | 64.3      |
| Nd1ii—Nd1—Rh1             | 120.592   | Rh1—Nd1—Nd1viii           | 115.7     |
| Rh1—Nd1—Rh1              | 82.432    | Rh1—Nd1—Nd1viii           | 115.741   |
| Rh1—Nd1—Rh1              | 51.481    | Rh1—Nd1—Nd1viii           | 64.259    |
| Nd1i—Nd1—Rh1i             | 128.519   | Rh1—Nd1—Nd1viii           | 60.296    |
| Nd1ii—Nd1—Rh1i            | 119.704   | Rh1—Nd1—Nd1viii           | 119.704   |
| Rh1—Nd1—Rh1i             | 60.296    | Rh1—Nd1—Nd1viii           | 180.0     |
| Rh1ii—Nd1—Rh1             | 59.408    | Rh1—Nd1—Nd1viii           | 119.704   |
| Rh1—Nd1—Rh1i              | 51.481    | Rh1—Nd1—Nd1viii           | 180.0     |
| Nd1i—Nd1—Rh1i             | 128.519   | Rh1—Nd1—Nd1viii           | 180.0     |
| Nd1ii—Nd1—Rh1i            | 119.704   | Rh1—Nd1—Nd1viii           | 180.0     |
| Rh1—Nd1—Rh1i              | 59.408    | Rh1—Nd1—Nd1viii           | 180.0     |
| Rh1v—Nd1—Rh1i             | 51.481    | Rh1—Nd1—Nd1viii           | 180.0     |
| Rh1vi—Nd1—Rh1i            | 128.519   | Rh1—Nd1—Nd1viii           | 180.0     |
| Rh1v—Nd1—Rh1i             | 51.481    | Rh1—Nd1—Nd1viii           | 180.0     |
| Rh1vi—Nd1—Rh1i            | 59.408    | Rh1—Nd1—Nd1viii           | 180.0     |
### Crystal data

SmRh$_3$B$_2$

$M_r = 480.70$

Hexagonal, P6/mmm

$a = 5.4438$ (2) Å

$c = 3.11901$ (12) Å

$V = 80.05$ (1) Å$^3$

$Z = 1$

$F(000) = 207$

$D_x = 9.972$ Mg m$^{-3}$

Cell parameters from 649 reflections

$\theta = 4.3$–$40.1^\circ$

$\mu = 32.61$ mm$^{-1}$

$T = 293$ K

Block, metallic

$0.06 \times 0.05 \times 0.02$ 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$^{-1}$

$\omega$ scans

Absorption correction: numerical

(CrysAlisPro; Rigaku OD, 2021)

$T_{\text{min}} = 0.324$, $T_{\text{max}} = 0.542$

696 measured reflections

129 independent reflections

128 reflections with $I > 2\sigma(I)$

$R_{\text{min}} = 0.011$

$\theta_{\text{max}} = 40.1^\circ$, $\theta_{\text{min}} = 4.3^\circ$

$h = -8 \rightarrow 9$

$k = -7 \rightarrow 7$

$l = -3 \rightarrow 5$

### Refinement

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.012$

$wR(F^2) = 0.032$

$S = 1.13$

129 reflections

9 parameters

0 restraints

$w = 1/[\sigma^2(F_c^2) + (0.0213P)^2 + 0.0484P]$

where $P = (F_c^2 + 2F_s^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta \rho_{\text{max}} = 1.76$ e Å$^{-3}$

$\Delta \rho_{\text{min}} = -0.97$ e Å$^{-3}$

Extinction correction: SHELXL-2016/6

(Sheldrick 2016),

$Fc^2 = kF^2[1 + 0.001xFc^2/\sin(2\theta)]^{1/4}$

Extinction coefficient: 0.034 (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      | Uiso/Usq |
|-----|--------|--------|--------|----------|
| 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)

|     | U₁₁ | U₂₂ | U₃₃ | U₁₂ | U₁₃ | U₂₃ |
|-----|-----|-----|-----|-----|-----|-----|
| 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, °)

|                  |       |                  |       |                  |       |
|------------------|-------|------------------|-------|------------------|-------|
| Sm1—Sm1          | 3.1190 (1) | Sm1—Rh1         |       | 3.1370 (1)       |
| Sm1—Sm1i         | 3.1190 (1) | Rh1—B1i         |       | 2.2140 (1)       |
| Sm1—Rh1i         | 3.1370 (1) | Rh1—B1ii        |       | 2.2140 (1)       |
| Sm1—Rh1v         | 3.1370 (1) | Rh1—B1iv        |       | 2.2140 (1)       |
| Sm1—Rh11         | 3.1370 (1) | Rh1—B1v         |       | 2.7219 (1)       |
| Sm1—Rh1          | 3.1370 (1) | Rh1—B1          |       | 2.7219 (1)       |
| Sm1—Rh1i         | 3.1370 (1) | Rh1—B1ii        |       | 2.7219 (1)       |
| Sm1—Rh1v         | 3.1370 (1) | Rh1—B1v         |       | 2.7219 (1)       |
| Sm1—Rh11         | 3.1370 (1) | Rh1—B1          |       | 2.7219 (1)       |
| Sm1—Rh1          | 3.1370 (1) | Rh1—Rh1i        |       | 3.1190 (1)       |
| Sm1—Rh1i         | 3.1370 (1) | Rh1—Rh1v        |       | 3.1190 (1)       |
| Sm1—Sm1i         | 180.0  | B1i—Rh1—Rh1v    |       | 52.069 (1)       |
| Sm1—Sm1—Sm1i     | 180.0  | B1i—Rh1—Rh1v    |       | 52.069 (1)       |
| Sm1—Sm1—Rh1v     | 60.189 (1) | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 119.811 (1) | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 119.811 (1) | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 60.189 (1)  | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 119.811 (1) | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 60.189 (2)   | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 119.811 (1) | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 128.6       | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 51.423 (1)   | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 60.189 (2)   | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 128.6       | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
| Sm1—Sm1—Rh1v     | 51.423 (1)   | B1i—Rh1—Rh1v    |       | 127.931 (1)      |
Rh1—Sm1—Rh1v 180.0
Sm1—Sm1—Rh1vi 60.189 (2)
Sm1—Sm1—Rh1vi 119.811 (1)
Rh1—Sm1—Rh1v 51.423 (1)
Rh1—Sm1—Rh1v 128.577 (1)
Rh1—Sm1—Rh1vi 97.428 (2)
Rh1—Sm1—Rh1vi 82.572 (2)
Sm1—Sm1—Rh1vii 119.811 (1)
Sm1—Sm1—Rh1vii 60.189 (2)
Rh1—Sm1—Rh1vii 128.577 (1)
Rh1—Sm1—Rh1vii 51.423 (1)
Rh1—Sm1—Rh1vii 82.572 (2)
Rh1—Sm1—Rh1vii 97.428 (2)
Sm1—Sm1—Rh1viii 119.811 (1)
Sm1—Sm1—Rh1viii 60.189 (1)
Sm1—Sm1—Rh1viii 119.811 (1)
Rh1—Sm1—Rh1viii 120.379 (3)
Rh1—Sm1—Rh1viii 59.621 (3)
Rh1—Sm1—Rh1viii 97.428 (2)
Rh1—Sm1—Rh1viii 82.572 (2)
Rh1—Sm1—Rh1viii 97.428 (2)
Rh1—Sm1—Rh1viii 82.572 (1)
Sm1—Sm1—Rh1ix 119.811 (1)
Sm1—Sm1—Rh1ix 60.189 (1)
Rh1—Sm1—Rh1ix 59.621 (3)
Rh1—Sm1—Rh1ix 120.379 (3)
Rh1—Sm1—Rh1ix 82.572 (2)
Rh1—Sm1—Rh1ix 97.428 (2)
Rh1—Sm1—Rh1ix 82.572 (1)
Rh1—Sm1—Rh1ix 97.428 (1)
Sm1—Sm1—Rh1x 119.811 (1)
Sm1—Sm1—Rh1x 60.189 (1)
Rh1—Sm1—Rh1x 59.621 (3)
Rh1—Sm1—Rh1x 120.379 (3)
Rh1—Sm1—Rh1x 82.572 (2)
Rh1—Sm1—Rh1x 97.428 (2)
Rh1—Sm1—Rh1x 82.572 (1)
Sm1—Sm1—Rh1xi 119.811 (1)
Sm1—Sm1—Rh1xi 60.189 (1)
Rh1—Sm1—Rh1xi 59.621 (3)
Rh1—Sm1—Rh1xi 120.379 (3)
Rh1—Sm1—Rh1xi 82.572 (2)
Rh1—Sm1—Rh1xi 97.428 (2)
Rh1—Sm1—Rh1xi 82.572 (1)
Rh1—Sm1—Rh1xi 97.428 (1)
Sm1—Sm1—Rh1xii 119.811 (1)
Sm1—Sm1—Rh1xii 60.189 (1)
Rh1—Sm1—Rh1xii 59.621 (3)
Rh1—Sm1—Rh1xii 120.379 (3)
Rh1—Sm1—Rh1xii 82.572 (2)
Rh1—Sm1—Rh1xii 97.428 (2)
Rh1—Sm1—Rh1xii 82.572 (1)
Rh1—Sm1—Rh1xii 97.428 (1)
Sm1—Sm1—Rh1xiii 119.811 (1)
Sm1—Sm1—Rh1xiii 60.189 (1)
Rh1—Sm1—Rh1xiii 59.621 (3)
Rh1—Sm1—Rh1xiii 120.379 (3)
Rh1—Sm1—Rh1xiii 82.572 (2)
Rh1—Sm1—Rh1xiii 97.428 (2)
Rh1—Sm1—Rh1xiii 82.572 (1)
Rh1—Sm1—Rh1xiii 97.428 (1)
Sm1—Sm1—Rh1xiv 119.811 (1)
Sm1—Sm1—Rh1xiv 60.189 (1)
Rh1—Sm1—Rh1xiv 59.621 (3)
Rh1—Sm1—Rh1xiv 120.379 (3)
Rh1—Sm1—Rh1xiv 82.572 (2)
Rh1—Sm1—Rh1xiv 97.428 (2)
Rh1—Sm1—Rh1xiv 82.572 (1)
Rh1—Sm1—Rh1xiv 97.428 (1)
Sm1—Sm1—Rh1xv 119.811 (1)
Sm1—Sm1—Rh1xv 60.189 (1)
Rh1—Sm1—Rh1xv 59.621 (3)
Rh1—Sm1—Rh1xv 120.379 (3)
Rh1—Sm1—Rh1xv 82.572 (2)
Rh1—Sm1—Rh1xv 97.428 (2)
Rh1—Sm1—Rh1xv 82.572 (1)
Rh1—Sm1—Rh1xv 97.428 (1)
Sm1—Sm1—Rh1xvi 119.811 (1)
Sm1—Sm1—Rh1xvi 60.189 (1)
Rh1—Sm1—Rh1xvi 59.621 (3)
Rh1—Sm1—Rh1xvi 120.379 (3)
Rh1—Sm1—Rh1xvi 82.572 (2)
Rh1—Sm1—Rh1xvi 97.428 (2)
Rh1—Sm1—Rh1xvi 82.572 (1)
Rh1—Sm1—Rh1xvi 97.428 (1)
Sm1—Sm1—Rh1xvii 119.811 (1)
Sm1—Sm1—Rh1xvii 60.189 (1)
Rh1—Sm1—Rh1xvii 59.621 (3)
Rh1—Sm1—Rh1xvii 120.379 (3)
Rh1—Sm1—Rh1xvii 82.572 (2)
Rh1—Sm1—Rh1xvii 97.428 (2)
Rh1—Sm1—Rh1xvii 82.572 (1)
Rh1—Sm1—Rh1xvii 97.428 (1)
Sm1—Sm1—Rh1xviii 119.811 (1)
Sm1—Sm1—Rh1xviii 60.189 (1)
Rh1—Sm1—Rh1xviii 59.621 (3)
Rh1—Sm1—Rh1xviii 120.379 (3)
Rh1—Sm1—Rh1xviii 82.572 (2)
Rh1—Sm1—Rh1xviii 97.428 (2)
Rh1—Sm1—Rh1xviii 82.572 (1)
Rh1—Sm1—Rh1xviii 97.428 (1)
Sm1—Sm1—Rh1xix 119.811 (1)
Sm1—Sm1—Rh1xix 60.189 (1)
Rh1—Sm1—Rh1xix 59.621 (3)
Rh1—Sm1—Rh1xix 120.379 (3)
Rh1—Sm1—Rh1xix 82.572 (2)
Rh1—Sm1—Rh1xix 97.428 (2)
Rh1—Sm1—Rh1xix 82.572 (1)
Rh1—Sm1—Rh1xix 97.428 (1)
Sm1—Sm1—Rh1xx 119.811 (1)
Sm1—Sm1—Rh1xx 60.189 (1)
Rh1—Sm1—Rh1xx 59.621 (3)
Rh1—Sm1—Rh1xx 120.379 (3)
Rh1—Sm1—Rh1xx 82.572 (2)
Rh1—Sm1—Rh1xx 97.428 (2)
Rh1—Sm1—Rh1xx 82.572 (1)
Rh1—Sm1—Rh1xx 97.428 (1)
Rh1 vii—Sm1—Rh1 x
128.577 (1) Rh1 viii—B1—Rh1 vii
75.862 (3)
Rh1 viii—Sm1—Rh1 x
51.423 (1) Rh1 viii—B1—Rh1 vii
138.425 (1)
Rh1 vii—Sm1—Rh1 x
128.577 (1) Rh1 viii—B1—Rh1 vii
138.425 (1)
Rh1 vii—Sm1—Rh1 x
180.0 Rh1 viii—B1—Rh1 vii
75.862 (3)
B1 vii—Rh1—B1 viii
89.561 (4) Rh1 viii—B1—Rh1 vii
138.425 (1)
B1 viii—Rh1—B1 viii
90.439 (4) Rh1 viii—B1—Rh1 vii
75.862 (2)
B1 viii—Rh1—B1 viii
90.439 (4) Rh1 viii—B1—Rh1 vii
138.425 (1)
B1 viii—Rh1—B1 vii
89.561 (4) Rh1 viii—B1—Rh1 vii
75.862 (3)
B1 viii—Rh1—B1 vii
180.0 Rh1 viii—B1—Rh1 vii
138.425 (1)
B1 viii—Rh1—B1 vii
52.069 (1) Rh1 viii—B1—Rh1 vii
89.562 (4)
B1 vii—Rh1—Rh1 xv
127.931 (1)

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