P3	−0.39733 (10)	0.91804 (9)	0.72381 (12)	0.0491 (3)
P4	−0.23517 (13)	1.10963 (8)	0.67693 (12)	0.0531 (3)
C1	0.2516 (4)	0.7417 (3)	0.6571 (3)	0.0345 (7)
O1	−0.0947 (2)	0.9479 (2)	0.8837 (2)	0.0343 (5)
O2	−0.0656 (3)	0.7393 (3)	0.4553 (3)	0.0543 (8)
O3	0.0827 (3)	0.7173 (2)	0.9471 (2)	0.0445 (6)
O4	−0.2393 (2)	0.8629 (2)	0.6993 (3)	0.0377 (5)
O5	−0.3650 (3)	0.9538 (2)	0.8765 (3)	0.0442 (6)
O6	0.3487 (3)	0.6915 (2)	0.6370 (3)	0.0521 (7)
O7	−0.1007 (3)	1.0253 (2)	0.6599 (3)	0.0403 (6)
C2	0.0878 (3)	0.7570 (2)	0.8477 (3)	0.0296 (6)
C3	−0.0031 (4)	0.7712 (3)	0.5470 (3)	0.0343 (7)
O8	0.2673 (3)	1.0133 (2)	0.6737 (4)	0.0630 (9)
C4	0.2015 (4)	0.9390 (3)	0.6812 (4)	0.0370 (7)
O9	−0.3720 (3)	1.0286 (3)	0.6504 (3)	0.0544 (8)
O10	−0.2257 (3)	1.1160 (2)	0.8382 (3)	0.0444 (6)

Table 2. *Selected geometric parameters (Å, °)*

Fe—C2	1.801 (3)	P2—O5	1.623 (3)
Fe—C1	1.805 (3)	P2—O1	1.663 (2)
Fe—P1	2.1233 (12)	O3—C2	1.136 (4)
P1—O1	1.608 (2)		
C2—Fe—C1	90.31 (15)	O5—P2—O1	99.16 (13)
C2—Fe—P1	89.22 (10)	P1—O1—P2	125.43 (14)
O1—P1—Fe	116.61 (9)	P2—O5—P3	127.8 (2)
O10—P2—O5	100.14 (15)		

Data collection: Enraf–Nonius diffractometer software. Cell refinement: Enraf–Nonius diffractometer software. Data reduction: *CADSHEL* (Kopf & Rübcke, 1993). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *SHELXL*93.

The authors thank the Deutsche Forschungsgemeinschaft (SFB 334) and the Fonds der Chemischen Industrie for kindly supporting this work.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: JZ1123). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Braga, D., Grepioni, F. & Orpen, A. G. (1993). *Organometallics*, **12**, 1481–1483.
Clade, J., Jansen, M., Engels, B. & Marian, C. M. (1995). *Z. Anorg. Allg. Chem.* **621**, 2065–2069.
Frick, F., Jansen, M., Bruna, P.-J. & Peyerimhoff, S. D. (1991). *Chem. Ber.* **124**, 1711–1714.
Jansen, M. & Möbs, M. (1984*a*). *Z. Anorg. Allg. Chem.* **514**, 39–48.
Jansen, M. & Möbs, M. (1984*b*). *Inorg. Chem.* **23**, 4486–4488.
Jansen, M. & Voss, M. (1981). *Angew. Chem.* **93**, 120–121.
Jansen, M., Voss, M. & Deiseroth, H.-J. (1981). *Angew. Chem.* **93**, 1023–1024.
Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Jost, K.-H. & Schneider, M. (1981). *Acta Cryst.* B**37**, 222–224.
Kopf, J. & Rübcke, H.-C. (1993). *CADSHEL. Program for Reduction of Enraf–Nonius CAD-*4 *Data*. Version 3.1. University of Hamburg, Germany.
Mühlhäuser, M., Engels, B., Marian, C. M., Peyerimhoff, S. D., Bruna, P.-J. & Jansen, M. (1994). *Angew. Chem.* **106**, 578–581.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Pierron, E. D., Wheatley, P. J. & Riess, J. G. (1966). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
Walker, M. L. & Mills, J. L. (1975). *Inorg. Chem.* **14**, 2438–2440.

Acta Cryst. (1996). C**52**, 2652–2655

A New Quaternary Borocarbide, $GdRh_2B_2C$

Jinhua Ye,[a] Toetsu Shishido,[b] Takashi Kimura,[a]
Takehiko Matsumoto[a] and Tsuguo Fukuda[b]

[a]*National Research Institute for Metals, 1-2-1 Sengen, Tsukuba, Ibaraki 305, Japan, and* [b]*Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba, Sendai 980, Japan. E-mail: ye@nrim.go.jp*

(*Received 17 April 1996; accepted 31 May 1996*)

Abstract

A new quaternary borocarbide, gadolinium dirhodium diboron carbide, has been synthesized by the flux method and its structure has been analyzed using single-crystal X-ray diffraction. The compound crystallizes as a derivative of the $ThCr_2Si_2$ structure type, as do many newly discovered superconducting compounds in the RT_2B_2C system (R = rare earth, T = transition metal). The structure consists of thick tetrahedrally coordinated Rh_2B_2 layers and GdC NaCl-type layers. These two atomic layers stack alternately along [001] *via* strong B—C bonds to form a three-dimensional network.

Comment

Since the discovery of superconductivity with T_c = 23 K in the Y–Pd–B–C system (Cava *et al.*, 1994), the interest in intermetallic compounds has been renewed and in the search for new quaternary borocarbides many new materials have been found for a variety of rare earth elements (R) and transition metals (T). Our group has studied the crystal chemistry and magnetic properties of the R–T–B ternary systems for many years, particularly for T = Co and Rh (Niihara, Shishido & Yajima, 1973; Shishido, Higashi, Kitazawa, Bernhard, Takei & Fukuda, 1994). Recently, we extended our search from the R–T–B ternary system to the R–T–B–C quaternary system and succeeded in the crystal growth of a new quaternary borocarbide, $GdRh_2B_2C$, using a copper flux.

The crystal structure of $GdRh_2B_2C$ is shown in Fig. 1. It may be viewed as a layered structure containing GdC NaCl-type layers and Rh_2B_2 slabs. Within the

GdC layer the Gd—C distance is 2.6510 (2) Å, showing less close packing compared with the atomic radii of metallic Gd (1.80 Å) and covalent C (0.77 Å) (Pearson, 1972). The Rh_2B_2 layers contain a square-planar Rh_2 array sandwiched between the B-atom planes. The Rh—Rh^{iii} in-plane distance is 2.6510 (2) Å, which is shorter than that found in metallic Rh (2.70 Å), suggesting strong metal–metal bonding within the layer. Each Rh atom is coordinated by four B atoms to form an RhB_4 tetrahedron with a B—Rh—B^{ii} bond angle of 105.13 (5)° and a B—Rh—B^{vii} angle of 118.6 (1)°, deviating from the ideal tetrahedral angle of 109.5°. The RhB_4 tetrahedra share edges to form the extended Rh_2B_2 slabs. The GdC and Rh_2B_2 layers are connected to each other by B—C bonds of 1.489 (3) Å, much shorter than the distance expected from the covalent radii of B (0.88 Å) and C.

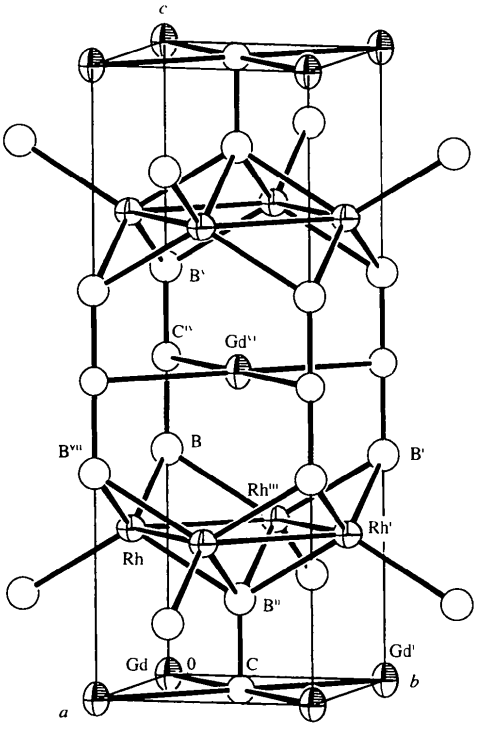

Fig. 1. *ORTEP*II (Johnson, 1976) illustration of $GdRh_2B_2C$. Displacement ellipsoids for Gd and Rh atoms are shown at 95% probability levels.

The structure of $GdRh_2B_2C$ is isomorphous with those of the recently discovered superconducting borocarbides RNi_2B_2C (Siegrist, Zandbergen, Cava, Krajewski & Peck, 1994). All these quaternary compounds may be viewed as having a modified $ThCr_2Si_2$-type structure (Ban & Sikirica, 1965) with the insertion of C atoms in the lanthanide layer. The $ThCr_2Si_2$ structure itself, interestingly, is common for many well known magnetic ternary borides RT_2B_2 (T = Co, Fe). We have investigated the phase stability of the compounds RRh_2B_2 and RRh_2B_2C synthesized by arc-melting for different rare earth elements (Ye, Shishido, Sasaki, Matsumoto & Fukuda, 1996) and have surveyed the RT_2B_2 and RT_2B_2C compounds other than T = Rh reported previously. The results suggested that the C atoms play an important role in the formation of the RT_2B_2C phase by adjusting the size of framework formed by the rare earth atoms, enabling transition metal atoms of different sizes to be accommodated in the $ThCr_2Si_2$ structure. The strong bonding between the B and C atoms in the title compound seems to make the modification of the $ThCr_2Si_2$ structure possible while leaving the overall structure unchanged. This is consistent with results for the RNi_2B_2C compounds (Siegrist, Cava, Krajewski & Peck, 1994), where the B—C distances range from 1.487 Å for R = La to 1.473 Å for R = Lu and are affected little by the variation in the radius of the lanthanide atom. The insertion of C atoms in the Gd layer results in the expansion of the B—B distance from 2.4 Å in the related $ThCr_2Si_2$-type compound $GdCo_2B_2$ (Niihara *et al.*, 1973) to 2.977 (5) Å in $GdRh_2B_2C$ and leads to a remarkable expansion of the *c* lattice parameter from 9.54 to 10.4122 (4) Å.

Besides the crystal chemistry role of the C atoms in the structure, it is interesting to consider the influence of the rare earth and transition metal elements on the stability of the RT_2B_2C phases. In the case of Ni, the RNi_2B_2C structure appears to accept all lanthanides readily and single crystals of RNi_2B_2C with R = La (the largest), Gd (intermediate) and Lu (the smallest) have been obtained. For Rh, however, only the largest, La, was reported to form the non-superconducting compound $LaRh_2B_2C$. Comparing the structural parameters of $LaRh_2B_2C$ with those of the title compound $GdRh_2B_2C$, little difference is found in the Rh—B and B—C^{iv} distances [2.212 (4), 1.519 (8) Å for the La compound and 2.181 (1), 1.489 (3) Å for the Gd compound, respectively]. However, the Rh—Rh distance decreases significantly from 2.7591 (2) Å in $LaRh_2B_2C$ to 2.6510 (2) Å in $GdRh_2B_2C$, the latter shorter than the distance expected from the metallic radius of Rh (2.70 Å). On the other hand, the Ni—Ni bond lengths are 2.6828 Å in $LaNi_2B_2C$ and 2.5279 Å in $GdNi_2B_2C$, both longer than calculated from the metallic radius of Ni (2.50 Å). Even in the compound containing the smallest lanthanide, Lu, the Ni—Ni bond length is 2.4493 Å, which is slightly shorter than expected from the metallic radius. From these crystallographic data, it is easy to understand why the RNi_2B_2C structure readily accepts all the lanthanides. Moreover, it could also be expected to be difficult to form the RRh_2B_2C phase with T = Rh or Gd, or with the smaller lanthanides. Indeed, we could only obtain multiphase samples by arc-melting syntheses, in spite of using a starting composition of 1:2:2:1 stoichiometry. The slight deficiency at the Rh site (or partial substitution of Rh atoms by smaller Cu atoms) revealed in the present structure analysis implies that the structure is strained by the presence of the large Rh atoms.

As expected from the approximate conservation of the B—C and T—B distances in the RT_2B_2C compounds, the TB_4 tetrahedron in the T_2B_2 layer tends to be deformed more from an ideal tetrahedron with increasing lanthanide size in response to the increase in the T—T distances. Electronic band-structure calculations for several Ni-based superconducting borocarbides and boronitrides such as $LuNi_2B_2C$ and $La_3Ni_2B_2N_3$ (Marttheiss, 1994; Marttheiss, Siegrist & Cava, 1994; Singh & Pickett, 1995) have revealed a common feature of a peak in the electronic density states near the Fermi level which is predominantly due to the contribution of the Ni 3*d* electrons. The calculations, as well as the fact that superconductivity is only observed for the smaller lanthanides in the RNi_2B_2C compounds, led to a suggestion that the superconductivity in borocarbide materials is influenced by the deformation of the TB_4 tetrahedron, *i.e.* the B—T—B angle. In $GdRh_2B_2C$, the B—T—B^{ii} angle is 105.13 (5)°, which is more deformed than the limiting value (107°) below which the RNi_2B_2C compounds are no longer superconducting (Siegrist, Cava, Krajewski & Peck, 1994). If the deformation in the TB_4 tetrahedra does predominantly affect the superconducting state, superconductivity is not expected in the new compound under ambient conditions. Larger single crystals would be desirable for the measurement of various physical properties of the compound and extensive investigation of the phases in the RT_2B_2C system is expected to result in a more definite understanding of the mechanism of the borocarbide superconductors.

Experimental

Single crystals of $GdRh_2B_2C$ were grown from a copper flux (Shishido, Ye, Sasaki, Matsumoto & Fukuda, 1996). The crystals have a thin plate-like habit with a maximum size of about 0.5 × 0.5 × 0.008 mm. The small crystal size and the small total amount of the sample limited the methods available for analysis. Electron-probe micro-analysis (EPMA) revealed the main component elements Gd, Rh, B and C, and slight contamination from the copper solvent. In addition to the difficulties caused by the small crystal size, the overlapping of the $K\alpha$ characteristic X-ray peak of C with the *MZ* and *Mg* lines from Rh and the *LN* line from Cu complicated the accurate determination of the chemical composition. The atomic ratio Gd:Rh:B:C was found to be close to 1:2:2:1, suggesting the composition $GdRh_2B_2C$.

Crystal data

$GdRh_2B_2C$
$M_r = 396.69$
Tetragonal
$I4/mmm$
$a = 3.7491$ (3) Å
$c = 10.4122$ (4) Å
$V = 146.35$ (1) Å^3
$Z = 2$
$D_x = 9.002$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 42.7$–$45.0°$
$\mu = 33.2$ mm^{-1}
$T = 292.0$ K
Thin plate
0.12 × 0.09 × 0.008 mm
Gold

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
Absorption correction: by integration from crystal shape
$T_{\min} = 0.1408$, $T_{\max} = 0.7537$
3013 measured reflections
374 independent reflections

340 observed reflections [$I > 3\sigma(I)$]
$R_{\rm int} = 0.13$
$\theta_{\max} = 60.0°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -25 \rightarrow 25$
3 standard reflections monitored every 100 reflections intensity decay: 1.35%

Refinement

Refinement on *F*
$R = 0.025$
$wR = 0.023$
$S = 1.450$
334 reflections
10 parameters
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{\max} = 0.000045$
$\Delta\rho_{\max} = 3.62$ e Å^{-3}
$\Delta\rho_{\min} = -3.72$ e Å^{-3}

Extinction correction: Zachariasen (1968) type 2 Gaussian isotropic
Extinction coefficient: 104 (12)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)*

$U_{\rm iso}$ for C and B, $U_{\rm eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$ for Gd and Rh.

	x	y	z	$U_{\rm iso}/U_{\rm eq}$
Gd	0	0	0	0.00681 (2)
Rh†	1/2	0	1/4	0.00648 (2)
C	1/2	1/2	0	0.0065 (4)
B	0	0	0.3570 (2)	0.0080 (4)

† Site occupancy = 0.934 (2).

Table 2. *Selected geometric parameters (Å, °)*

Gd—Gd^{i}	3.7491 (3)	Rh—B	2.181 (1)
Gd—Rh	3.2078 (1)	Rh—C	3.2078 (1)
Gd—B^{ii}	3.041 (1)	B—C^{iv}	1.489 (3)
Gd—C	2.6510 (2)	B—B^{v}	2.977 (5)
Rh—Rh^{iii}	2.6510 (2)		
Rh—Gd^{vi}—Rh^{iii}	48.814 (2)	Gd^{vi}—Rh—B^{ii}	84.96 (6)
Rh—Gd^{vi}—Rh^{i}	71.518 (6)	Rh^{iii}—Rh—B	52.56 (3)
Rh—Gd^{vi}—C^{iv}	65.593 (3)	Rh^{iii}—Rh—B^{vii}	127.44 (3)
B—Rh—B^{ii}	105.13 (5)	Rh—B^{ii}—Rh^{iii}	74.87 (5)
B—Rh—B^{vii}	118.6 (1)	Rh—B^{ii}—Rh^{i}	118.6 (1)
Gd^{vi}—Rh—B	65.51 (4)	Rh—B^{ii}—C	120.72 (6)

Symmetry codes: (i) $x, 1+y, z$; (ii) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii) y, x, z; (iv) $x-\frac{1}{2}, y-\frac{1}{2}, \frac{1}{2}+z$; (v) $x, y, 1-z$; (vi) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}+z$; (vii) $1+x, y, z$.

Because of the thin plate-like habit and very brittle nature of the crystals, it was difficult to shape the sample into a favorable form without destroying its single-crystal nature, although a spherical shape would have been desirable in view of the high absorption coefficient of the compound. In the present study, a small fragment cut from a larger piece of crystal was used for intensity measurements. The single-crystal nature of the sample was checked and the possible space groups were determined using a precession camera. After careful observation of various diffraction patterns, only *hkl* reflections with $h + k + l = 2n + 1$ were recognized to be systematically absent, indicating the space groups $I\bar{4}2m$, $I\bar{4}m2$, $I422$, $I4mm$ and $I4/mmm$. The space group was determined to be $I4/mmm$ through structure analyses based on all these space groups, as described below. Neither long-range superstructure reflections nor streaking were observed.

Reflections with $2\theta < 80°$ were measured in the full reciprocal sphere and reflections with $80 < 2\theta < 120°$ were measured in half the reciprocal sphere. Reflection data were corrected for Lorentz–polarization effects and absorption. The intensities of symmetrically equivalent reflections were then averaged, giving $R_{\rm int} = 0.13$, indicating the difficulty in correcting for absorption given the very large absorption coefficient and extremely anisotropic shape of the crystal. To reduce the influence of the inadequate absorption correction on the results of structure analyses, reflections were collected in the largest multiplicity as described above.

Full-matrix least-squares refinement was carried out using the $ThCr_2Si_2$ structure (Ban & Sikirica, 1965) as the initial structure model. The Gd, Rh and B atoms were placed at the crystallographic positions of the Th, Cr and Si atoms, *i.e.* the 2*a*, 4*d* and 4*e* sites of the space group $I4/mmm$, respectively, while the C atoms were placed at the 2*b* site in the centre of the Gd plane. By varying the scale factor, the isotropic extinction, the atomic positions and anisotropic displacement parameters for Gd and Rh, the least-squares refinement converged to unweighted and weighted agreement factors, *R* and *wR*, of 0.039 and 0.061, respectively. Furthermore, the occupancy parameter of Rh was refined to 0.934 (2), revealing a slight deviation from full occupancy of the 4*d* sites and leading to further convergence to $R = 0.030$ and $wR = 0.023$. The slight deficiency at the Rh site might suggest partial substitution of Rh by Cu, the presence of which had been revealed by EPMA. Refinements of the occupancies of other sites did not indicate any deficiency and *R* and *wR* were not reduced further. Six strong reflections in the low angle region of $2\theta < 30°$ which might be strongly affected by absorption and extinction were excluded in the final stage of the structure refinement. This refinement resulted in the final *R* and *wR* values of 0.025 and 0.023, and produced an F_o *versus* F_c list in very good agreement. The final difference-electron density map had maxima and minima of 3.62 and -3.72 e Å^{-3} in the vicinity of the Gd atoms.

Possible deviation from centrosymmetry was examined by full-matrix least-squares refinement in all the possible non-centrosymmetric space groups ($I\bar{4}2m$, $I\bar{4}m2$, $I422$ and $I4mm$). No shift in the structural parameters larger than the errors was observed and no significant improvement in the results of the structure analysis were obtained. Therefore, the space group of $GdRh_2B_2C$ was determined as $I4/mmm$, the highest symmetry space group among those possible.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1992). Program(s) used to refine structure: *TEXSAN LS*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *TEXSAN FINISH*.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: BR1145). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Ban, Z. & Sikirica, M. (1965). *Acta Cryst.* **18**, 594–599.

Cava, R. J., Takagi, H., Batlogg, B., Zandbergen, H. W., Krajewski, J. J., Peck, W. F. Jr, Dover, R. B., Felder, R. J., Siegrist, T., Mizuhashi, K., Lee, J. O., Eisaki, H., Carter, S. A. & Uchida, S. (1994). *Nature*, **367**, 146–148.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Marttheiss, L. F. (1994). *Phys. Rev. B*, **49**, 13279–13282.

Marttheiss, L. F., Siegrist, T. & Cava, R. J. (1994). *Solid State Commun.* **91**, 587–590.

Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Molecular Structure Corporation (1992). *TEXSAN. Single Crystal Structure Analysis Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Niihara, K., Shishido, T. & Yajima, S. (1973). *Bull. Chem. Soc. Jpn*, **46**, 1137–1140.

Pearson, W. B. (1972). In *The Crystal Chemistry and Physics of Metals and Alloys*. New York: John Wiley.

Shishido, T., Higashi, I., Kitazawa, H., Bernhard, J., Takei, H. & Fukuda, T. (1994). *Jpn. J. Appl. Phys. Ser.* **10**, 142–143.

Shishido, T., Ye, J., Sasaki, T., Matsumoto, T. & Fukuda, T. (1996). In preparation.

Siegrist, T., Cava, R. J., Krajewski, J. J. & Peck, W. F. Jr (1994). *J. Alloys Compd.* **216**, 135–139.

Siegrist, T., Zandbergen, H. W., Cava, R. J., Krajewski, J. J. & Peck, W. F. Jr (1994). *Nature*, **367**, 254–256.

Singh, D. J. & Pickett, W. E. (1995). *Phys. Rev. B*, **51**, 8668–8671.

Ye, J., Shishido, T., Sasaki, T., Matsumoto, T. & Fukuda, T. (1996). In preparation.

Zachariasen, W. H. (1968). *Acta Cryst.* A**24**, 212–216.

Acta Cryst. (1996). C**52**, 2655-2660

$Na_8H_{18}[\{Er_3O(OH)_3(H_2O)_3\}_2Al_2(Nb_6O_{19})_5].40.5H_2O$

HARUO NARUKE AND TOSHIHIRO YAMASE

Research Laboratory of Resources Utilization, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226, Japan. E-mail: hnaruke@res.titech.ac.jp

(Received 4 March 1996; accepted 4 June 1996)

Abstract

The $[\{Er_3O(OH)_3(H_2O)_3\}_2Al_2(Nb_6O_{19})_5]^{26-}$ anion in the title compound, octadecahydrogen octasodium dialuminopentanonacontaoxobis(triaquatrihydroxooxotrierbio)triacontaniobate(26−)-water (1/40.5), is com-

Acta Crystallographica Section C
ISSN 0108-2701 © 1996