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Novel Ternary Oxobromides with Ta_6 Clusters and Rare Earths: The Synthesis of (RE)$Ta_6Br_{13}O_3$ (RE = Rare Earth) and the Crystal Structure of $LuTa_6Br_{13}O_3$

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Crystallochemistry of the novel oxobromides (RE)$Ta_6Br_{13}O_3$ with RE = Sm to Lu (except Eu and Yb) is reported. All these compounds, which exhibit 14 valence electrons per Ta_6 cluster, are isotypic with $ScNb_6Cl_{13}O_3$ with the space group $I4_122$. The structure of $LuTa_6Br_{13}O_3$ has been determined from single crystal X-ray diffraction: $a = 9.383(1)$ Å and $c = 54.60(1)$ Å, $R = 0.050$ and $R_w = 0.054$ for 755 symmetry-independent reflections. For this compound, the (Ta_6L_{18}) units (L = Br and O), in which the Ta_6 cluster is very distorted, are linked together by four bridging bromines to form pseudo-helices of units. The lutetium is five-coordinated at a small site formed by three oxygen and two bromine atoms belonging to three adjacent units. The formula developed for this compound is $Lu(Ta_6Br_9^{i}O_3^{i})Br_2^{a}Br_{4/2}^{a-a}$. These structural results allow discussion of the influence of interatomic distances on the potential properties of these novel ternary tantalum oxobromides in relation to the oxidation state of the cluster.

INTRODUCTION

In the last few years, we have developed a new series of halides based on Ta_6 or Nb_6 clusters and rare earths which exhibit two structure types, labelled $KLuNb_6Cl_{18}$, and $CsLuNb_6Cl_{18}$.[1–3] In all these compounds of the general formula $A_x(RE)M_6X_{18}$ (A = monovalent cation, RE = rare earth; M = Nb or Ta; X = Cl, Br ; x = 0, 1, 2), the M_6 cluster can exhibit magnetic or non-magnetic behaviour, depending on its oxidation state (16 or 15 valence electrons per cluster : VEC). The rare earth, lying in a distorted halogen octahedron, is located far from the M6 cluster, which cannot favour magnetic interactions.[4]

We have tried to reduce the distance between the rare earth and the M_6 cluster by introducing a smaller ligand, such as oxygen, around the cluster. Indeed, in these last years, ternary Nb_6 cluster oxides have been isolated, for instance $Mg_3Nb_6O_{11}$,[5] ANb_8O_{14} (A = K, La)[6] or quaternary $Na_3Al_2Nb_{34}O_{64}$, $Na(Si,Nb)Nb_{10}O_{19}$[7] and recently $Rb_4Al_2Nb_{35}O_{70}$,[8] in which the cluster is edge-capped by oxygen in a similar way as with halogens. The corresponding oxides seem not to be developed in the tantalum cluster chemistry. However, we have succeeded in obtaining the first Ta_6 cluster oxobromides with a rare earth, the formula of which is $(RE)Ta_6Br_{13}O_3$ (RE = rare earth). This series is isotypic with the structure type $ScNb_6Cl_{13}O_3$ recently determined by us[9]; it belongs to the tetragonal symmetry with the space group $I4_122$.

In this paper, we report our recent results on the crystallochemistry of the new $(RE)Ta_6Br_{13}O_3$ oxobromides and we present the crystal structure of $LuTa_6Br_{13}O_3$ determined by single-crystal X-ray diffraction as described below.

EXPERIMENTAL

Synthesis and X-ray Characterization of $(RE)Ta_6Br_{13}O_3$

The $(RE)Ta_6Br_{13}O_3$ compounds (RE = Sm to Lu, except Eu and Yb) have been prepared by solid state reaction from stoichiometric amounts of rare earth oxides (Saint-Gobain 3N), Ta_2O_5 (Ventron, purity 99.5%), $TaBr_5$ (Ventron, purity 99.9%) and Ta powder (Ventron, purity m2N8). The mixture, handled in dry atmosphere, is pressed in the form of a pellet and placed in an evacuated sealed silica tube. It is heated at 700 °C with some pieces of tantalum foil.

Single crystals of these ternary tantalum oxobromides are very difficult to grow and are usually of low quality. Thus, it has not been easy to select a single crystal suitable for structural determination by X-ray diffraction. A similar observation was already made during the synthesis of the $A_x(RE)Ta_6Br_{18}$ bromides, in contrast to the corresponding niobium cluster compounds for which single crystals of good quality were easily obtained.[3]

The unit-cell constants of all these tantalum oxobromides have been determined by a least squares fit from the X-ray powder patterns, using Si as internal standard, recorded with an INEL CPS 120 diffractometer, equipped with a position-sensitive detector (Cu Kα1 radiation).

Data Collection for Structural Determination of $LuTa_6Br_{13}O_3$

A $LuTa_6Br_{13}O_3$ crystal (0.07 x 0.07 x 0.05 mm^3) obtained directly during the synthesis was selected for structural determination. The unit-cell constants were determined by least squares refinement on setting angles of 24 reflections: a = 9.383(1) Å and c = 54.60(1) Å.

The intensities were recorded at room temperature with a NONIUS CAD-4 four circle diffractometer using graphite-monochromated Mo Kα radiation. Conditions limiting the possible reflections are: hkl, $h + k + l = 2n$ and $00l$, $l = 4n$. All reflections within a sphere defined by $\theta < 30°$ were examined by the ω-scan mode ($1.0 + 0.35 \tan \theta$). 4075 intensities were measured ($0 < h < 13$, $0 < k < 13$, $0 < l < 77$). After averaging ($R_{\text{int}} = 0.043$), 755 observations with $I > 2.5\ \sigma(I)$ were used for the refinement. DIFABS absorption corrections were applied.[10]

TABLE I

Positional parameters and their estimated standard deviations for $LuTa_6Br_{13}O_3$
$B\text{eq} = 4/3\ \Sigma\Sigma\ a_i\ a_j\ B_{ij}$

Atom	Position	x	y	z	$B/\text{Å}^2$
Ta1	16g	0.5907(3)	0.3794(3)	0.83964(4)	1.65(4)
Ta2	16g	0.5788(3)	0.3628(3)	0.78505(5)	1.73(5)
Ta3	16g	0.1872(3)	0.1149(3)	0.31358(5)	1.75(4)
Br1	16g	0.3828(7)	0.2010(6)	0.8481(1)	2.0(1)
Br2	16g	0.1763(7)	0.5210(7)	0.7793(1)	2.3(1)
Br3	16g	0.3625(6)	0.1899(6)	0.7817(1)	2.2(1)
Br4	16g	0.3046(7)	0.8242(7)	0.8129(1)	2.3(1)
Br5	8c	1/2	1/2	0.7467(2)	2.6(2)
Br6	16g	0.0552(7)	0.2537(8)	0.8209(1)	2.8(1)
Br7	8f	1/4	0.762(1)	7/8	3.2(2)
Br8	8e	−0.8284(7)	0.828	0	2.3(1)
O1	8c	1/2	1/2	0.8671(9)	1(1)
O2	16g	0.230(3)	0.513(4)	0.8382(6)	0.8(7)
Lu	8c	1/2	1/2	0.90428(7)	2.09(8)

Intensity data treatment and refinement calculations were performed using the MOLEN programs[11] on a Digital Micro Vax 3100. The structure was solved in the $I4_122$ space group by isotypy with $ScNb_6Cl_{13}O_3$.[9] The full-matrix least-squares refinement on F with anisotropic thermal parameters converged with $R = 0.050$ and $R_w = 0.054$, where $1/w = 1/4[\sigma^2(I) + (0.05I)^2]/I$, with $S = 0.950$ and $(\Delta/\sigma)_{\max} = 0.03$. The scattering factors were taken from Ref. 12. The final difference Fourier synthesis gives $\Delta\rho_{\max} = 3.0(7)$ e Å^{-3} and $\Delta\rho_{\min} = -1.5(7)$ e Å^{-3}. The enantiomer has been checked and does not procure a better result. The final atomic parameters are reported in Table I. The interatomic distances and angles are summarized in Table II. Additional informations, anisotropic thermal parameters, observed and calculated structure factors, can be obtained on request from the Editorial Office.

TABLE II

Interatomic distances/Å and angles/° for $LuTa_6Br_{13}O_3$

Ta_6 cluster			
Ta1-Ta1	2.832(6)	Ta1-Ta1-Ta3	63.9(1)
Ta1-Ta2	2.987(4)	Ta1-Ta1-Ta3	57.2(1)
Ta1-Ta3	2.780(4)	Ta2-Ta2-Ta3	61.13(9)
Ta1-Ta3	2.972(4)	Ta2-Ta2-Ta3	59.13(9)
Ta2-Ta2	2.968(6)	Ta2-Ta1-Ta3	62.8(1)
Ta2-Ta3	3.009(4)	Ta2-Ta1-Ta3	59.3(1)
Ta2-Ta3	2.950(4)	Ta1-Ta2-Ta3	60.1(1)
Ta1-Ta2	4.155(4)	Ta1-Ta2-Ta3	55.2(1)
Ta3-Ta3	4.122(4)		
$(Ta_6Br_9{}^iO_3{}^i)$ unit			
Ta1-Br1	2.612(7)	Ta1-O1	2.06(4)
Ta1-Br4	2.596(8)	Ta1-O2	1.97(3)
Ta2-Br2	2.562(7)	Ta3-O2	1.96(4)
Ta2-Br3	2.605(7)		
Ta2-Br4	2.569(8)	shortest other distances in the unit:	
Ta2-Br5	2.568(9)	Br2-Br2	3.33(1)
Ta3-Br1	2.640(8)	O1-O2	2.99(4)
Ta3-Br2	2.600(7)	Br6-O2	3.08(4)
Ta3-Br3	2.570(7)		
Ta-ligand in apical position			
bridges: Ta1-Br7	2.780(6)	Ta1-Br7-Ta1	122.9(4)
Ta2-Br8	2.764(4)	Ta2-Br8-Ta2	152.7(4)
terminal: Ta3-Br6	2.743(7)		
Lutetium environment			
Lu-O1	2.03(5)	O2-Lu-O2	158.(2)
Lu-O2	2.20(3)	O1-Lu-O2	100.8(9)
Lu-Br6	2.727(8)	Br6-Lu-O1	119.7(2)
		Br6-Lu-O2	76.5(9)
		Br6-Lu-O2	92.(1)
		Br6-Lu-Br6	120.5(3)
Shortest other distances			
Ta3-Lu	3.585(1)	Ta1-Ta1	4.883
Ta1-Lu	3.803(2)	Ta2-Ta2	5.372
Ta1-Lu	4.017(1)	Lu-Lu	5.678

RESULTS

Crystallochemistry of (RE)$Ta_6Br_{13}O_3$

The series of compounds (RE)$Ta_6Br_{13}O_3$ (RE = Sm to Lu) is isotypic with tetragonal $ScNb_6Cl_{13}O_3$, space group $I4_122$. We have refined the unit-cell constants of the compounds reported in Figure 1. Their unit-cell parameters range from a = 9.472(4) Å, c = 55.33(3) Å for $SmTa_6Br_{13}O_3$ to a = 9.383(1) Å, c = 54.60(1) Å for $LuTa_6Br_{13}O_3$. The variation of the volume closely correlates with the evolution of the ionic radius of the trivalent rare earth, as commonly observed for other compounds of the (RE)M_6X_{18} type.[13] Thus far we have not succeeded in obtaining the corresponding compounds with europium and ytterbium. Indeed, in the niobium or tantalum cluster chemistry, these two rare earths usually form special compounds due to their two possible oxidation states.

Crystal Structure of $LuTa_6Br_{13}O_3$

The structure of $LuTa_6Br_{13}O_3$, isotypic with $ScNb_6Cl_{13}O_3$ (Figure 2), is built of Ta_6L_{18} (L = Br and O) units in which the Ta_6 cluster is edge-capped by nine bromine and three oxygen atoms which are ordered. Six additional

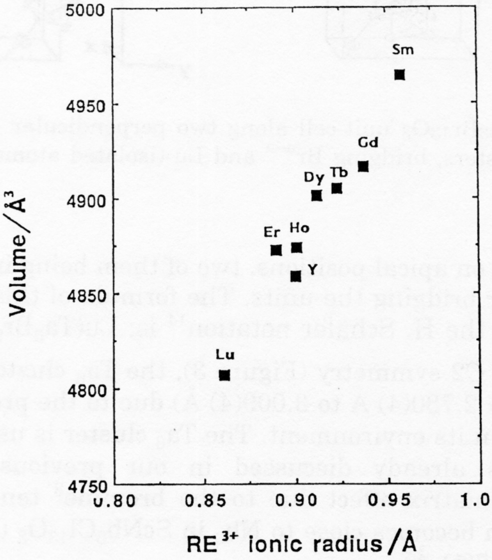

Figure 1. Evolution of the unit-cell volume *versus* the ionic radius of trivalent rare earths for (RE)$Ta_6Br_{13}O_3$. The ionic radius of the trivalent six-coordinated rare earths given in Ref. 16 have been used.

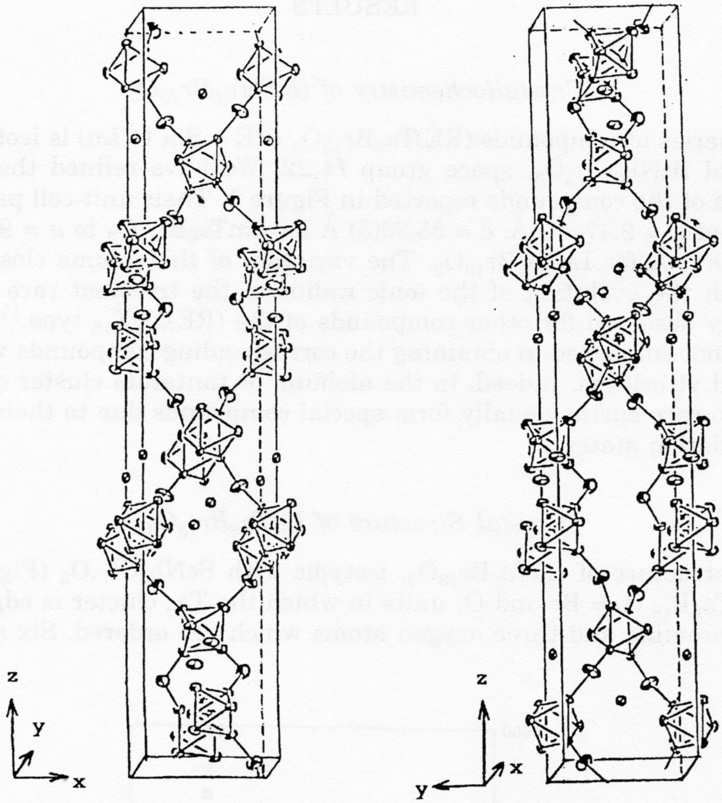

Figure 2. The $LuTa_6Br_{13}O_3$ unit-cell along two perpendicular directions. For more clarity only Ta_6 clusters, bridging Br^{a-a} and Lu (isolated atoms) are represented.

bromine atoms lie on apical positions, two of them being in terminal position and the other four bridging the units. The formula of this compound, developed according to the H. Schäfer notation[14] is: $Lu(Ta_6Br_9{}^iO_3{}^i)Br_2{}^aBr_{4/2}{}^{a-a}$.

In this unit of *C*2 symmetry (Figure 3), the Ta_6 cluster is very distorted (Ta-Ta distances = 2.780(4) Å to 3.009(4) Å) due to the presence of both oxygen and bromine in its environment. The Ta_6 cluster is usually smaller than the Nb_6 one, as already discussed in our previous works,[15] but in $LuTa_6Br_{13}O_3$ the matrix effect due to the bromine[3] tends to increase the cluster size, which becomes close to Nb_6 in $ScNb_6Cl_{13}O_3$ (Nb-Nb distances = 2.805(1) Å to 3.007(1) Å).

The $Ta\text{-}Br^i$ and $Ta\text{-}O^i$ distances are consistent with the corresponding distances observed in $ScNb_6Cl_{13}O_3$ and close to the $Ta\text{-}Br^i$ and Ta-O distances in $CsErTa_6Br_{18}$ or tantalum oxides, respectively. Like in $ScNb_6Cl_{13}O_3$, the termi-

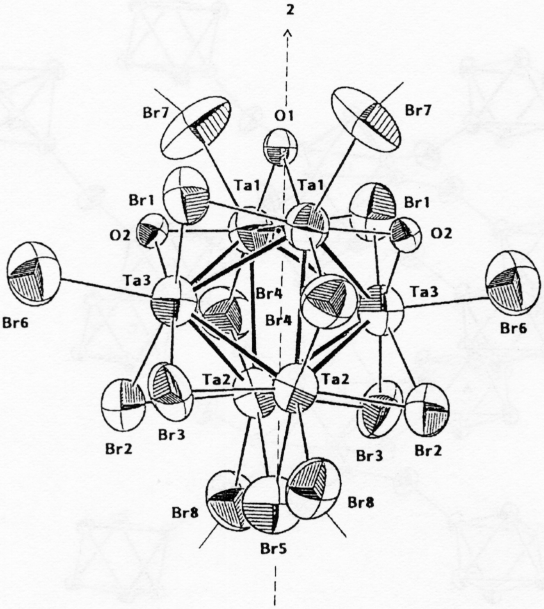

Figure 3. The $(Ta_6Br_9{}^iO_3{}^i)Br_2{}^aBr_{4/2}{}^{a-a}$ unit.

nal Ta-Br^a and bridging Ta-Br^{a-a} distances are close to each other, in contrast to the corresponding distances in binary cluster compounds ($M\text{-}X^a < M\text{-}X^{a-a}$) which are usually very different; this feature is due to the influence of the RE^{3+} cations which are bound to the Br^a atoms as described below.

The units are linked together by four bridging bromines (Br7 and Br8), with two very different Ta-Br^{a-a}-Ta angles: 122.9(4)° and 152.7(4)°; these angles are comparable to those in $ScNb_6Cl_{13}O_3$. This linkage forms pseudo-helical units, their axes being perpendicular to each other (Figure 4a and b), which is a very original feature in cluster chemistry.

The lutetium atoms are located in that part of the structure where the $Br7^{a-a}$ bridging bromines are concentrated (Figure 4b) with Lu-Br7 = 3.757 Å, while the distance between Lu and the other bridging bromines is very large: Lu-Br8 = 6.805 Å. If one considers the first coordination sphere, each lutetium lies at a five coordinated-site of $C2$ symmetry, formed by three O^i and two Br^a atoms (Lu-O = 2.03(5) Å and 2.20(3) Å, and Lu-Br = 2.727(8) Å) (Figure 5), belonging to three adjacent units. This site is unique for a rare earth, usually six-coordinated at a distorted octahedral site of halogens in $A(RE)M_6X_{18}$[9,13] halides, or at more complex sites in the rare earth oxides or in ternary cluster oxides, for instance 12-coordinated in $LaNb_8O_{14}$.[6]

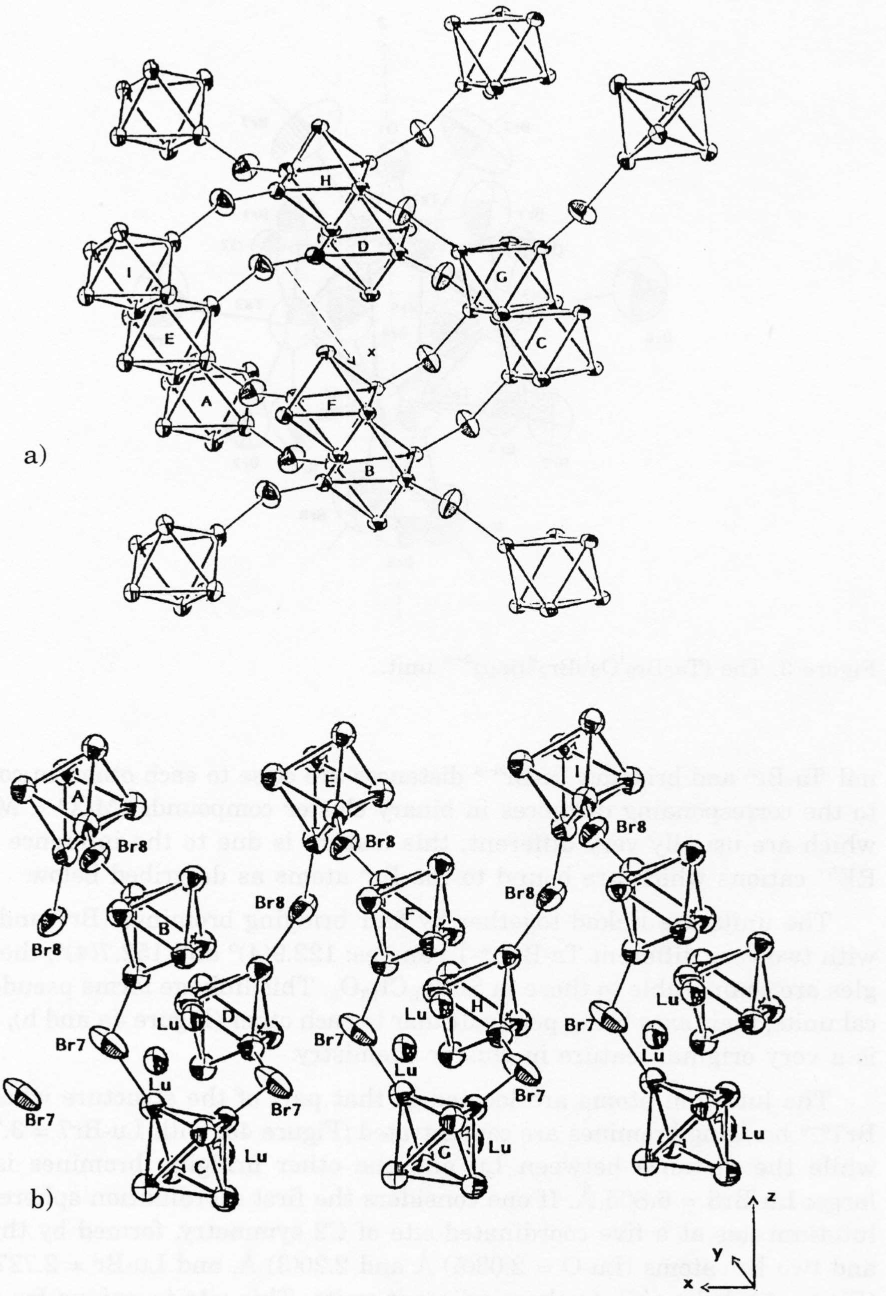

Figure 4. a) Representation of the boundings between the clusters *via* the Br^{a-a} bromines, forming a helix of units. A to I label indicates the successive linkage (perspective view), b) The same helix along a perpendicular direction (perspective view).

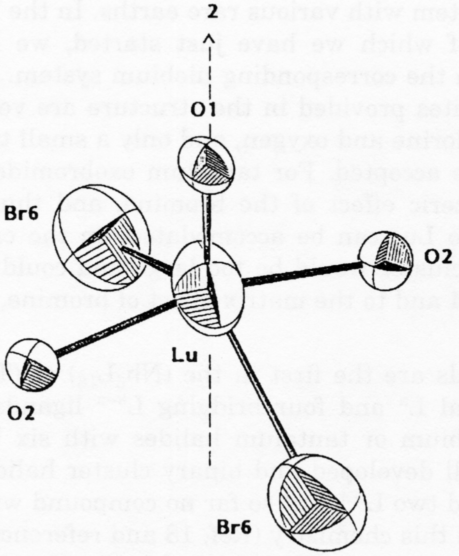

Figure 5. The lutetium environment.

Even if the size of the Ta_6 cluster is close to that of Nb_6, the RE sites formed betweeen the units are larger than in $ScNb_6Cl_{13}O_3$, due to the steric effect of the large bromine atoms, which is not compensated in the stacking by the replacement of Nb by Ta. This results in a RE-M distance larger in $LuTa_6Br_{13}O_3$ (Lu-Ta = 3.585(1) Å than in $ScNb_6Cl_{13}O_3$ (Sc-Nb = 3.391(1) Å), but this distance stays much shorter than the RE-M distance in $A(RE)M_6Br_{18}$, for instance in $CsErTa_6Br_{18}$ (Er-Ta = 5.231(1) Å).[15]

DISCUSSION AND CONCLUSIONS

These $(RE)M_6X_{13}O_3$ are the first oxohalides obtained so far in cluster chemistry based on M_6L_{18} units, and the first cluster compounds with halogen ligands exhibiting 14 electrons per M_6 cluster which have been synthesized at high temperature using the procedures of solid state chemistry. The presence of oxygen allows to stabilize such an oxidation state for the M_6 cluster; indeed, VEC = 14 corresponds to a stable cluster oxidation state in ternary cluster oxides.[17]

In the RE-Nb-Cl-O system, only one compound of this $I4_122$ structure type has been obtained so far: $ScNb_6Cl_{13}O_3$ while in the RE-Nb-Br-O system no such compound has been isolated. In contrast, for tantalum chemistry, as we have pointed out above, several isotypical $I4_122$ compounds exist in the RE-Ta-Br-O system with various rare earths. In the RE-Ta-Cl-O system, the investigation of which we have just started, we have only obtained $ScTa_6Cl_{13}O_3$, like in the corresponding niobium system. Indeed, for the oxochlorides, the RE sites provided in the structure are very small due to the presence of both chlorine and oxygen, and only a small trivalent cation such as scandium can be accepted. For tantalum oxobromides, the RE sites are large due to the steric effect of the bromine, and thus rather large rare earths (RE = Sm to Lu) can be accomodated. In the case of niobium oxobromides, the Nb_6 cluster would be too large and could not be established, due to the VEC = 14 and to the matrix effect of bromine, as we have already discussed.[15]

These compounds are the first in the (Nb_6L_{18}) or (Ta_6L_{18}) chemistry to exhibit two terminal L^a and four bridging L^{a-a} ligands in the same compound. Indeed, niobium or tantalum halides with six L^a or six L^{a-a} have been previously well developed and binary cluster halides such as Nb_6Cl_{14} exhibit four L^{a-a} and two L^{i-a}, but so far no compound with both L^a and L^{a-a} has been isolated in this chemistry (Ref. 18 and references therein). The latter type of linkage, which usually leads to sheets of units when two L^a and four L^{a-a} are present, is well known in the molybdenum and rhenium cluster chemistry as well as in quaternary zirconium cluster halides, for instance in Mo_6X_{12},[19] $Re_6Se_6Cl_6$[20] and $Na_4Zr_6Cl_{16}Be$,[21] respectively. In $(RE)M_6X_{13}O_3$, the great dissymmetry of the unit leads to a particular linkage in the helix *via* these four X^{a-a} halogens, instead of sheets of units.

Of special interest is the fact that this $(RE)Ta_6Br_{13}O_3$ series can be obtained for a number of rare earth ions, including the magnetic ones, in contrast to the RE-M-Cl-O system where only scandium compounds $ScM_6Cl_{13}O_3$ exist. The RE-Ta distances are short, as discussed above, and we would expect some magnetic interactions between the rare earths and the Ta_6 cluster if we could turn it into a magnetic cluster. To obtain such a behaviour, a possibility is to insert hydrogen inside the cluster in a similar way as in Nb_6I_{11}.[22] Some experiments are now in progress, and encouraging results have been already obtained.

We have just started investigations of the RE-Ta-I-O system in order to search for compounds with the $I4_122$ structure type. No new compounds of this type have been synthesized. It is probably due to the size of the cluster which is expected to be too large in the iodine cluster chemistry even with a VEC = 14; moreover, it would request the presence of two terminal I^a iodines, a situation which has never been obtained so far for tantalum or niobium cluster iodides by solid state chemistry synthesis. Indeed, only one binary tantalum cluster iodide with I^{a-a} and I^{i-a} ligands, Ta_6I_{14} (VEC = 16 and four I^{a-a}) synthesized at high temperature, is well established.[23] In the RE-Ta-Br-I-O system, we have recently evidenced some bromo-iodides isotypic with $LuTa_6Br_{13}O_3$. The study of this system is now in progress, but one can suppose that the iodine should occupy the bridged I^{a-a} position since iodine in inner position would require a too large deformation. This disposition would manage larger RE sites in the $I4_122$ structure type, allowing also the insertion of a rather large rare earth, such as cerium.

Supplementary Materials. – Crystallographic data (excluding structure factors which are available from the authors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-109/68-781. Copies of the data can be obtained on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK. (Fax: 44 (0) 1223-336033; E-mail: teched@chemcrys.cam.ac.uk).

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SAŽETAK

Novi ternarni oksobromidi s klusterom Ta_6 i elementima rijetkih zemalja. Sinteza $(RE)Ta_6Br_{13}O_3$ (RE = rijetke zemlje) i kristalna struktura $LuTa_6Br_{13}O_3$

Stéphane Cordier, Christiane Perrin i Marcel Sergent

Opisana je kristalokemija novih oksobromida $(RE)Ta_6Br_{13}O_3$ s RE = Sm do Lu (osim Eu i Yb). Svi ti spojevi sadrže 14 elektrona po klusteru Ta_6 i istog su tipa kao i spoj $ScNb_6Cl_{13}O_3$, prostorne grupe $I4_122$. Struktura $LuTa_6Br_{13}O_3$ određena je rentgenskom difrakcijom na monokristalu: $a = 9.383(1)$ Å i $c = 54.60(1)$ Å, $R = 0.050$ i $R_w = 0.054$, za 755 simetrijski neovisnih refleksa. U ovom spoju jedinice Ta_6L_{18} (L = Br i O) u kojima je kluster Ta_6 jako deformiran, povezane su međusobno preko četiri atoma broma (u mostu) tvoreći jedinice pseudo-heliksa. Lutecij ima kooridnaciju pet; tri atoma kisika i dva atoma broma pripadaju trima susjednim klusterskim jedinicama. Kemijska formula toga spoja jest $Lu(Ta_6Br_9^{i}O_3^{i})Br_2^{a}Br_{4/2}^{a-a}$. Ovi strukturni rezultati dopuštaju raspravu o utjecaju međuatomskih udaljenosti na moguća svojstva novih ternarnih oksobromida tantala u ovisnosti o oksidacijskom stanju klustera.