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Hydrokenomicrolite, $(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$, a new microlite-group mineral from Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil

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Abstract

Hydrokenomicrolite, $(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$ or ideally $\square_2Ta_2[O_4(OH)_2](H_2O)$, is a new microlite-group mineral approved by the CNMNC (IMA 2011-103). It occurs as an accessory mineral in the Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil. Associated minerals are: microcline, albite, quartz, muscovite, spodumene, "lepidolite", cassiterite, tantalite-(Mn), monazite-(Ce), fluorite, "apatite", beryl, "garnet", epidote, magnetite, gahnite, zircon, "tourmaline", bityite, and other microlite-group minerals under study. Hydrokenomicrolite occurs as euhedral octahedral crystals, occasionally modified by rhombododecahedra, untwinned, from 0.2 to 1.5 mm in size. The crystals are pinkish brown and translucent; the streak is white, and the luster is adamantine to resinous. It is non-fluorescent under ultraviolet light. Mohs hardness is 4½–5, tenacity is brittle. Cleavage is not observed; fracture is conchoidal. The calculated density is 6.666 g/cm^3. The mineral is isotropic, n_{calc} = 2.055. The infrared spectrum contains bands of O-H stretching vibrations and H-O-H bending vibrations of H_2O molecules. The chemical composition (n = 3) is [by wavelength-dispersive spectroscopy (WDS), H_2O calculated from crystal-structure analysis, wt%]: CaO 0.12, MnO 0.27, SrO 4.88, BaO 8.63, PbO 0.52, La_2O_3 0.52, Ce_2O_3 0.49, Nd_2O_3 0.55, Bi_2O_3 0.57, UO_2 4.54, TiO_2 0.18, SnO_2 2.60, Nb_2O_5 2.18, Ta_2O_5 66.33, SiO_2 0.46, Cs_2O 0.67, H_2O 4.84, total 98.35. The empirical formula, based on 2 cations at the B site, is $[\square_{0.71}(H_2O)_{0.48}Ba_{0.33}Sr_{0.27}U_{0.10}Mn_{0.02}Nd_{0.02}Ce_{0.02}La_{0.02}Ca_{0.01}\ Bi_{0.01}Pb_{0.01}]_{\Sigma 2.00}$ $(Ta_{1.75}Nb_{0.10}Sn_{0.10}Si_{0.04}Ti_{0.01})_{\Sigma 2.00}[(O_{5.77}(OH)_{0.23}]_{\Sigma 6.00}[(H_2O)_{0.97}Cs_{0.03}]_{\Sigma 1.00}$. The strongest eight X-ray powder-diffraction lines [d in Å(I)(hkl)] are: 6.112(86)(111), 3.191(52)(311), 3.052(100)(222), 2.642(28)(400), 2.035(11)(511)(333), 1.869(29)(440), 1.788(10)(531), and 1.594(24)(622). The crystal structure refinement (R_1 = 0.0363) gave the following data: cubic, $Fd\bar{3}m$, a = 10.454(1) Å, V = 1142.5(2) Å^3, Z = 8. The $Ta(O,OH)_6$ octahedra are linked through all vertices. The refinement results and the approximate empirical bond-valences sums for the positions A (1.0 v.u.) and Y' (0.5 v.u.), compared to valence calculations from electron microprobe analysis (EMPA) and ranges expected for H_2O molecules, confirm the presence of H_2O at the A(16d) site and displaced from the Y(8b) to the Y'(32e) position. The mineral is characterized by H_2O dominance at the Y site, vacancy dominance at the A site, and Ta dominance at the B site.

Keywords: Hydrokenomicrolite, new mineral, Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil, pyrochlore supergroup, microlite group, crystal structure

Introduction

Hydrokenomicrolite, $(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$ or ideally $\square_2Ta_2[O_4(OH)_2](H_2O)$, from Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil, is a new mineral (IMA 2011-103) named according to the nomenclature system for the pyrochlore supergroup of minerals approved by IMA-CNMNC (Atencio et al. 2010). The general formula of the pyrochlore-supergroup minerals is $A_{2-m}B_2X_{6-w}Y_{1-n}$, where m = 0 to 1.7, w = 0 to 0.7, n = 0 to 1 (Lumpkin and Ewing 1995). In hydrokenomicrolite, the A site is dominated by vacancies, the B site is dominated by Ta, and the Y site is dominated by H_2O. The discredited mineral species "bariomicrolite" (Hogarth 1977), identical with "rijkeboerite" (van der Veen 1963), is too poor in Ba to correspond to the name "bariomicrolite". It apparently has a vacancy at the dominant A position and H_2O as a predominant component at the Y position, and as such is also probably hydrokenomicrolite. The "bariomicrolite" studied by Beurlen et al. (2005) is probably also hydrokenomicrolite (Atencio et al. 2010). Type material is deposited in the collections of the Museu de Geociências, Instituto

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de Geociências, Universidade de São Paulo, Rua do Lago, 562, 05508-080 São Paulo, SP, Brazil, registration number DR725.

Occurrence

The mineral occurs as an accessory phase in the Volta Grande pegmatite (21°10′08.6″S 44°36′01.3″W), Nazareno, Minas Gerais, Brazil, and the associated minerals are: microcline, albite, quartz, muscovite, spodumene, "lepidolite", cassiterite, tantalite-(Mn), monazite-(Ce), fluorite, "apatite", beryl, "garnet", epidote, magnetite, gahnite, zircon, "tourmaline", bityite, and other microlite-group minerals under study (Heinrich 1964; Francesconi 1972; Lagache and Quéméneur 1997). The hydrokenomicrolite crystals were collected in a heavy minerals concentrate, so the paragenetic position cannot be established. Other crystals of different colors, also corresponding to microlite group minerals occur in the same concentrate. Some of these crystals are formed by the association between Ca-Na-dominant microlite (under study) and hydrokenomicrolite, which may suggest that hydrokenomicrolite is an alteration product of Ca-Na-dominant microlite. The crystals used for characterization of hydrokenomicrolite, however, are homogeneous, not containing, therefore, association with other species. The pegmatite belongs to the Sn-Ta-rich São João del Rei Pegmatite Province. The Volta Grande granitic pegmatite is associated with Transamazonian granites (Early Proterozoic) hosted by the Archean greenstone belt of the Rio das Mortes Valley, which is situated at the southern border of the São Francisco Craton, in Minas Gerais, Brazil (Lagache and Quéméneur 1997). The pegmatite bodies, which are usually large (up to 1200 × 40 m), show a dominant intermediate zone containing spodumene, microcline, albite, and quartz, with an irregular border of an aplitic facies surrounded by an extensive metasomatic aureole with "zinnwaldite", phlogopite, and holmquistite. The spodumene-rich core zone is continuous or segmented, and also contains lenses of "lepidolite". The main rock type that hosts the pegmatite is an amphibole schist. This pegmatite is characterized by their high Rb and Li content (Lagache and Quéméneur 1997).

Habit and physical properties

Hydrokenomicrolite occurs as octahedra, occasionally modified by rhombododecahedra, untwinned, from 0.2 to 1.5 mm in size (Fig. 1). The crystals are pinkish brown with a white streak. The luster is adamantine to resinous. The mineral is translucent. It is non-fluorescent under ultraviolet light. Mohs hardness is 4½–5; Van der Veen (1963) observed VHN_{100} = 485 to 498 kg/mm^2 with 3 measurements for "bariomicrolite", a mineral that probably is the same as hydrokenomicrolite. The tenacity is brittle. Cleavage was not observed; fracture is conchoidal. The calculated density is 6.666 g/cm^3 based on the empirical formula and unit-cell parameters obtained from the single-crystal X-ray diffraction data.

The mineral is isotropic. Refractive index calculated from the Gladstone-Dale relationship based on the empirical formula is n_{calc} = 2.055 (higher than that of available immersion liquids). Van der Veen (1963) observed reflectivity of 12.8 to 13.6, mean 13.2, which is equivalent to n_D = 2.141 (three measurements in air relative to a glass standard with a reflectivity of 8.3%, refractive index 1.809, for "bariomicrolite" (see comments for "bariomicrolite" above).

Figure 1. Hydrokenomicrolite from Nazareno, Minas Gerais, Brazil.

Infrared data

The infrared (IR) absorption spectrum of hydrokenomicrolite (Fig. 2) was obtained for a powdered sample (mixed with anhydrous KBr and pelletized) using BRUKER ALPHA FTIR spectrometer, at the resolution of 4 cm^{-1} and the number of scans equal to 16. A pure KBr-disk was used as a reference sample.

The (IR) spectrum of hydrokenomicrolite contains bands of O-H stretching vibrations (2900–3700 cm^{-1}) and H-O-H bending vibrations of H_2O molecules (1640 and 1620 cm^{-1}). H_2O molecules form hydrogen bonds of different types (from weak to very strong). Weak bands at 890 and 1015 cm^{-1} correspond to stretching vibrations of SiO_4 tetrahedra and/or Ta···O-H bending vibrations. All other bands in the range 360–700 cm^{-1} are due to vibrations of the microlite-type framework.

Composition of hydrokenomicrolite

The composition of hydrokenomicrolite was determined using an Oxford INCA Wave 700 electron microprobe (WDS mode, 20 kV, 20 nA, electron beam rastered on the area 300 × 300 nm^2). H_2O was calculated from the crystal structure data; H_2O determined by gas chromatography of the products obtained by heating at 1200 °C is 6.74 wt%. However, part of this water probably is not a structural component, but is absorbed in macropores. Mean analytical results (n = 3) are given in Table 1. The contents of F, Na, P, S, Cl, K, Fe, and Th are below detection limits.

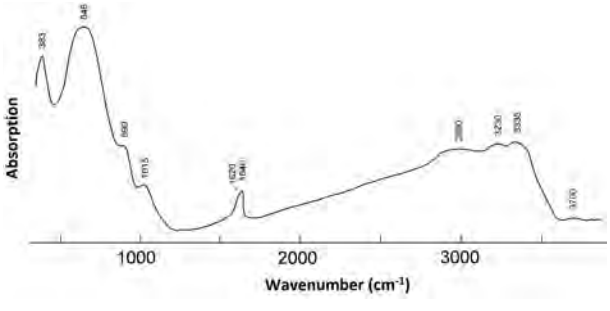

Figure 2. IR spectrum of hydrokenomicrolite.

TABLE 1. Chemical analyses of hydrokenomicrolite (n = 3)

	wt%	Range	Microprobe standard
CaO	0.12	n.d.–0.20	wollastonite
MnO	0.27	0.22–0.36	Mn
SrO	4.88	4.61–5.37	SrF_2
BaO	8.63	8.40–8.83	BaF_2
PbO	0.52	0.39–0.59	PbTe
La_2O_3	0.52	0.50–0.54	$LaPO_4$
Ce_2O_3	0.49	0.37–0.62	$CePO_4$
Nd_2O_3	0.55	0.49–0.62	$NdPO_4$
Bi_2O_3	0.57	0.40–0.74	Bi
UO_2	4.54	3.91–4.88	UO_2
TiO_2	0.18	0.14–0.27	Ti
SnO_2	2.60	2.40–2.98	Sn
Nb_2O_5	2.18	1.71–2.47	Nb
Ta_2O_5	66.33	65.76–67.39	Ta
SiO_2	0.46	n.d.-0.72	SiO_2
Cs_2O	0.67	0.60–0.76	CsCl
H_2O*	4.84		
Total	98.35		

* Calculated from the structure refinement.

The empirical formula, based on 2 cations at the *B* site is $[\square_{0.71}(H_2O)_{0.48}Ba_{0.33}Sr_{0.27}U_{0.10}Mn_{0.02}Nd_{0.02}Ce_{0.02}La_{0.02}Ca_{0.01}Bi_{0.01}Pb_{0.01}]_{\Sigma 2.00}(Ta_{1.75}Nb_{0.10}Sn_{0.10}Si_{0.04}Ti_{0.01})_{\Sigma 2.00}[O_{5.77}(OH)_{0.23}]_{\Sigma 6.00}[(H_2O)_{0.97}Cs_{0.03}]_{\Sigma 1.00}$. The simplified formula is $(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$. The only charge-balanced end-member variant of this formula is $\square_2Ta_2[O_4(OH)_2](H_2O)$.

CRYSTAL STRUCTURE DETERMINATION

Powder X-ray diffraction data were obtained using a Siemens D5000 diffractometer equipped with a Göbel mirror and a position-sensitive detector. Data (for Cu*K*α, 40 kV and 40 mA) are given in Table 2. Unit-cell parameters refined from powder data (space group $Fd\bar{3}m$) are $a = 10.5733(9)$ Å, $V = 1182.0(3)$ Å^3, and $Z = 8$.

A pinkish brown crystal with the dimensions 0.197 × 0.170 × 0.104 mm^3 was used for the structural investigation. X-ray diffraction measurements were made with an Enraf-Nonius Kappa-CCD diffractometer with graphite-monochromated Mo*K*α (λ = 0.71073 Å) radiation. Data were collected up to 64° in 2θ. Final unit-cell parameters are based on 331 reflections with the index ranges $-15 \le h \le 15$, $-11 \le k \le 11$, $-9 \le l \le 9$. The COLLECT program (Enraf-Nonius 1997–2000) was used for data collection, and the integration and scaling of the reflections were performed with the HKL Denzo-Scalepack system of programs (Otwinowski and Minor 1997). Face-indexed numerical absorption corrections were applied (Coppens et al. 1965). The structure was solved using the Patterson method with SHELXS-97 (Sheldrick 2008). The model was refined on the basis of F^2 by full-matrix least-squares procedures. The data obtained are: cubic, space group $Fd\bar{3}m$, $a = 10.454(1)$ Å, $V = 1142.4(2)$ Å^3, and $Z = 8$. The details concerning data collection procedures, structure determination and refinement are summarized in Table 3. Other crystallographic data are listed in Tables 4 and 5. More details, including anisotropic ADPs, are in the CIF file (deposit item CSD-424480).

TABLE 2. X-ray powder-diffraction data for hydrokenomicrolite

d_{obs} (Å)	d_{calc} (Å)	I_{obs} (%)	*h k l*
6.112	6.104	86	1 1 1
3.191	3.188	52	3 1 1
3.052	3.052	100	2 2 2
2.642	2.643	28	4 0 0
2.424	2.426	7	3 3 1
2.035	2.035	11	5 1 1
	2.035		3 3 3
1.869	1.869	29	4 4 0
1.788	1.787	10	5 3 1
1.613	1.612	7	5 3 3
1.594	1.594	24	6 2 2
1.527	1.526	7	4 4 4
1.480	1.481	7	7 1 1
	1.481		5 5 1
1.376	1.377	6	7 3 1
	1.377		5 5 3
1.213	1.213	5	6 6 2
1.182	1.182	5	8 4 0

Note: Indexed with $a = 10.5733$ Å.

TABLE 3. Crystal data and details of structure refinement

Temperature (K)	293(2)
Crystal color	pinkish brown
Crystal size (mm)	0.197 × 0.170 × 0.104
Formula weight	577.2
Crystal system	Cubic
Space group	$Fd\bar{3}m$ (227)
Unit-cell dimension *a*	10.454(1) Å
Unit-cell volume *V*	1142.4(2) Å^3
Z	8
Density (calculated)	6.7 g/cm^3
Absorption coefficient	38.097
F(*000*)	1941
Reflections collected/unique	331/121
Parameters	16 ($R_{int} = 0.056$)
Goodness-of-fit on F^2	1.191
Final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0363$, $wR_2 = 0.1009$
Largest diff. peak and hole	1.75 and –2.16 e·Å^{-3}

The holotype pyrochlore structures have all atoms occupying special positions (*A* = 16*d*, *B* = 16*c*, *X* = 48*f*, and *Y* = 8*b*) in $Fd\bar{3}m$. The *A* position was initially assumed to be *A*(16*d*) and the occupation was constrained by the microprobe obtained compositional data, as $(Ba_{0.33}Sr_{0.27}U_{0.10}Ce_{0.02}La_{0.02}Mn_{0.02}Nd_{0.02}Bi_{0.01}Ca_{0.01}Pb_{0.01})_{\Sigma 0.81}$. The *X* and *B* sites were set at full occupancy and *B* was constrained to the value obtained from the compositional data, $(Ta_{1.75}Nb_{0.10}Sn_{0.10}Si_{0.04}Ti_{0.01})_{\Sigma 2.00}$. The *Y* position was refined anisotropically and located at Wyckoff position 8*b*. The Cs content was constrained by microprobe analysis and H_2O presence was also checked. The H_2O occupancy presented positional disorder at 8*b* during refinement while Cs behaved as expected. Attempts to refine *Y*′ at 32*e* were done setting anisotropic ADPs. The position 32*e* was modeled partially with an occupation factor of 0.24 as the maximum occupation factor of 8*b* is equal to 1. However, a difference Fourier map showed a large negative maximum, –3.48 e·Å^{-3}, in the vicinity of the *Y*′ site, and a large positive maximum, 2.96 e·Å^{-3}, in the vicinity of the *Y* site. Thus positions 8*b* and 32*e* were modeled to be fractionally occupied by (Cs, H_2O) and H_2O, respectively. Refinement of this model converged to $R_1 = 0.0363$, $wR_2 = 0.1009$. The final model exhibits $[Cs_{0.03}(H_2O)_{0.32}]$ at 8*b*, $(H_2O)_{0.65}$ at 32*e* and $(H_2O)_{0.48}$ at 16*d*, and gave a total H_2O content in the mineral of 1.45 pfu = (0.48 + 0.97 pfu). Charge balance was maintained by replacing O by OH at the *X*(48*f*) position $[(O_{5.77}(OH)_{0.23}]_{\Sigma 6.00}$ (Figs. 3 and 4).

The maximum amount of H_2O in the pyrochlore structure is controlled by the cation occupancy of the *A* site; the maximum

[1] Deposit item AM-13-019, CIFs. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

TABLE 4. Wyckoff positions, site occupancies, atom coordinates, and equivalent isotropic displacement parameters (Å^2) in hydrokenomicrolite

	Wyckoff	Occupancy	x	y	z	U_{eq} (Å^2)
A	16*d*	0.64	1/2	1/2	1/2	0.0556(17)
B	16*c*	1	0	0	0	0.0306(6)
X	48*f*	1	0.3191(14)	1/8	1/8	0.038(3)
Y	8*b*	0.35	3/8	3/8	3/8	0.051(14)
Y′	32*e*	0.16	0.747(4)	0.747(4)	0.747(4)	0.051(14)

TABLE 5. Selected bond lengths and bond valences of the refined hydrokenomicrolite structure

Bond	Bond length	BV (v.u)	Σ	Valence from EMPA
A(16*d*)-*X*(48*f*)	2.644(10)	0.119 (x6)	0.714	
A(16d)-Y(8b)	2.2633(2)	0.106 (x2)	0.212	
A(16*d*)-*Y′*(32*e*)	2.59(6)	0.022 (x6)	0.132	
Σ			1.058	1.080
B(16*c*)-*X*(48*f*)	1.984(5)	0.828 (x6)	4.968	
Σ			4.968	4.926
X(48*f*)-*A*(16*d*)	2.644(10)	0119 (x2)	0.238	
X(48*f*)-*B*(16*c*)	1.984(5)	0.807 (x2)	1.614	
Σ			1.852	1.962
Y(8b)-A(16d)	2.2633(2)	0.106 (x4)	0.424	
Σ			0.424	0.000
Y′(32*e*)-*A*(16*d*)	2.59(6)	0.022 (x3)	0.066	
Σ			0.066	0.000

H_2O content ranges from 1.00 H_2O pfu for ideal pyrochlores (two *A* cations pfu, i.e., $m = 0$) to 1.75 H_2O pfu for *A*-deficient pyrochlores (no *A* cations, i.e., $m = 2$) (Ercit et al. 1994). Low *A* site cation content, high-displacement parameters for the *Y* site constituents, and the site splitting sometimes observed for the *Y* site indicate that the "O" on the *Y* sites can be H_2O. Ercit et al. (1994) found that H_2O molecules were actually displaced away from the ideal 8*b* *Y* sites, and partially occupied higher-multiplicity positions nearby. Displacements were by 0.57 Å along approximately <112> directions to 96*g* *Y″*, or a similar distance along <111> to 32*e* *Y″*-positions. A 192*i* position (*Y‴*) very close to *Y′* was also located by Philippo et al. (1995). Such displacements allow optimal distances between *A* and *Y* site species to be maintained.

For pyrochlore-supergroup minerals $A_2B_2X_6Y$, in which *A* and *B* are cations, and *X* and *Y* are anions, there are no stereochemical constraints for the maximum occupancies of the *A* and *Y* sites. However, for pyrochlore-supergroup minerals with H_2O in both the *A* and *Y* sites, the maximum occupancies of both sites are limited owing to the short separation between the ideal *A* and *Y* sites, which is in the neighborhood of 2.3 Å (Ercit et al. 1994). Partial occupancy of the *A* site and positional disorder of H_2O at *A* and *Y* sites permit acceptable O···O separations for neighboring H_2O groups in pyrochlore. Ercit et al. (1994) found that positional disorder can result in eight fractionally occupied *A′* sites around each *A* site, displaced from the ideal site by about 0.11 Å along <111> directions. Five of the eight are too close to the offset *Y′* and *Y″* positions to represent stable O···O separations for H_2O groups; however, three of the eight subsites are sufficiently distant to correspond to realistic intermolecular distances (averaging 2.74 Å). Philippo et al. (1995) reported a different displacement scheme, in which H_2O partially occupied *A″*-sites displaced from *A* by 0.75 Å along <100>. For synthetic cation-free *A*-site pyrochlore, the maximum H_2O content pfu may be limited by the need to avoid close H_2O···H_2O distances. If there is one H_2O group pfu in the *Y* site, then there can be only 3/8 H_2O groups in the *A* site. This constraint translates to a maximum of 1.75 H_2O pfu for *A* cation-free pyrochlore. Previous refinements of the structures of H_2O-bearing pyrochlore-supergroup minerals (e.g., Groult et al. 1982) have shown the presence of H_2O only in the vicinity of the *Y* site. As no synthetic or natural pyrochlore has been found with all H_2O ordered at *A*, we presume that the *Y* site and its displaced variants are the preferred locations for H_2O, and that H_2O only enters the *A* sites if *Y* cannot accommodate more H_2O. The maximum amount of H_2O pfu in the pyrochlore structure is thus $1 + (3m/8)$ where *m* indicates the vacancy at the *A* site.

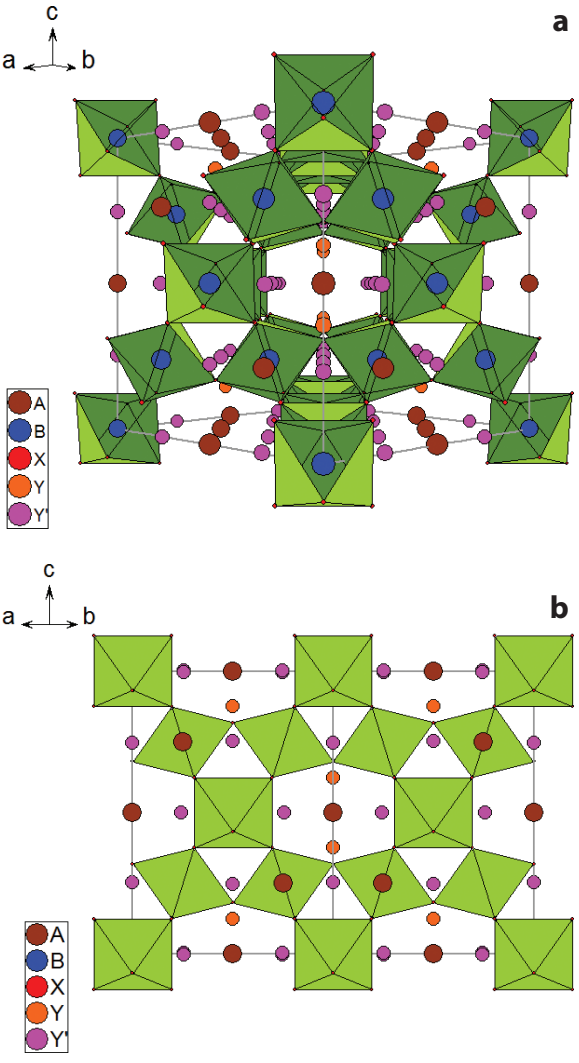

FIGURE 3. Hydrokenomicrolite structure.

The total amount of H_2O in the mineral is insufficient for the predominance of H_2O in the *A* site, but H_2O is predominant in the *Y* and *Y′* sites (Table 4). Empirical bond-valences (Table 5) were calculated using the parameters published by Brown and Altermatt (1985). These values agree with the composition of the *X* anion site chosen to balance the chemical formula and confirm the presence of molecular H_2O at the *Y′* site. The final refinement is consistent with a cubic $Fd\bar{3}m$ structure and the

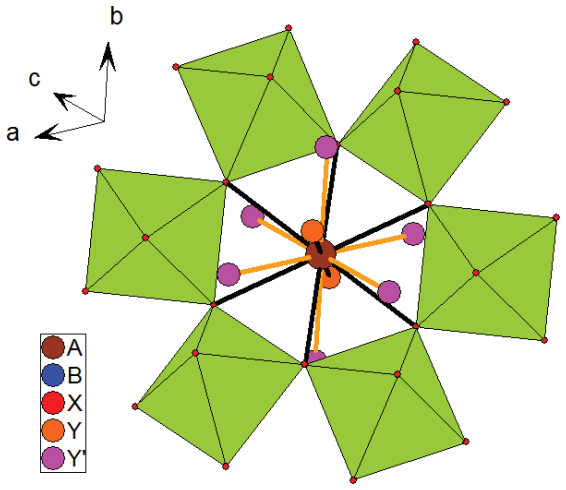

FIGURE 4. Relationship between *Y* and *Y*′ sites.

charge-balanced empirical formula is $[\square_{0.71}(H_2O)_{0.48}(Ba_{0.33}Sr_{0.27}U_{0.10}Ce_{0.02}La_{0.02}Mn_{0.02}Nd_{0.02}Bi_{0.01}Ca_{0.01}Pb_{0.01})_{\Sigma 0.81}]_{\Sigma 2.00}(Ta_{1.75}Nb_{0.10}Sn_{0.10}Si_{0.04}Sn_{0.10}Ti_{0.01})_{\Sigma 2.00}[O_{5.77}(OH)_{0.23}]_{\Sigma 6.00}[Cs_{0.03}(H_2O)_{0.97}]_{\Sigma 1.00}$.

Regardless of the absence of tetrahedral sites suitable for Si incorporation in the pyrochlore structure, octahedral Si is possible. The occurrence of Si in pyrochlore group minerals was discussed by Atencio et al. (2010). Perhaps hydrokenomicrolite could be an example of a mineral with mixed occupancies of a key domain. Unlike sites sensu stricto, domains can be defined as microregions in the unit cell that can host several alternative sites having, in a general case, different coordination numbers, as in eudialyte-group minerals (Nomura et al. 2010). Thus, an NbO_6 octahedron would be "replaced" by a SiO_4 tetrahedron. When Nb is in the microregion, the coordination number would be 6 and when Si is in the microregion, it would be 4.

Another argument in favor of the possible presence of SiO_4 tetrahedra in hydrokenomicrolite comes from the fact that there are several minerals (titano- and niobosilicates, or, more precisely, oxosilicates) whose crystal structures are regular interstratifications of pyrochlore-type and silicate modules (blocks) (Chakhmouradian and Mitchell 2002). The best known example is natrokomarovite, but several other minerals have such structures as well [e.g., diversilite-(Ce), ilímaussite-(Ce), fersmanite] (Pekov et al. 2004). By analogy, one can suppose that pyrochlore-supergroup minerals can contain, locally, two- or three-dimensional structural defects irregularly distributed within individual crystals. Such "block isomorphism" is not a rare phenomenon for minerals whose crystal structures are based on frameworks with relatively low density [cf. two local situations in the unit cell of manganoeudialyte (Nomura et al. 2010)]. If this supposition is correct, Si-bearing defects cannot be detected by single-crystal structural analysis. However, high-resolution electron microscopy might be useful to solve this problem.

ACKNOWLEDGMENTS

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0	8	12	33381.15	29632.77	3802.86	o
2	8	12	105.87	650.64	933.04	o
4	8	12	24439.22	20642.04	1047.18	o
1	1	13	8713.60	8020.68	725.51	o
1	3	13	6523.19	6643.90	647.00	o
3	3	13	10566.29	8428.85	1077.76	o
1	5	13	5484.05	5480.75	747.42	o
3	5	13	6387.44	6420.90	953.45	o

5	5	13	2850.06	2365.60	1898.47	o
1	7	13	5543.04	4697.37	943.16	o
3	7	13	3384.35	3691.08	1009.27	o
5	7	13	3415.15	4454.31	3128.14	o
0	2	14	41.69	1174.31	1094.45	o
2	2	14	35093.40	31933.25	2488.61	o
2	4	14	57.94	1360.21	722.52	o
4	4	14	34.43	1868.27	1515.83	o
0	6	14	3.18	685.00	1459.71	o
2	6	14	20658.01	16435.55	1879.04	o
1	1	15	4946.40	4627.03	1531.24	o
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2011-11-11 # Formatted by publCIF
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_publ_contact_author_name    'Andrade, Marcelo Barbosa de'

_publ_contact_author_email       mabadean@terra.com.br
_publ_contact_author_phone       '55(11)33739881'

_publ_requested_journal          'American Mineralogist'
#------------------ TITLE AND AUTHOR LIST-------------------------------------#
_publ_section_title
;
CRYSTAL <i>STRUCTURE</i> OF HYDROKENOMICROLITE VOLTA GRANDE PEGMATITE, MINAS
GERAIS, BRAZIL
;
loop_
_publ_author_name
;
Marcelo B. ANDRADE;Daniel ATENCIO; Nikita Chuvanov;Javier ELLENA
;
#------------------  SECTION 2. COMPOUND(S) DETAILS -------------------------#
_audit_creation_date                    2011-11-11
_audit_creation_method                  'WinGX routine CIF_UPDATE'

#------------------ CHEMICAL INFORMATION -------------------------------------#
_chemical_name_systematic
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Barium Strontium Uranium Cerium Lanthanum Magnesium Neodymium Bismuth
Calcium Lead Tantalum Silicon Niobium Tin Titanium Cesium
Oxide Hydroxide
;
_chemical_formula_structural
;
((H2 O)0.48 Ba0.33 Sr0.27 U0.10 Ce0.02 La0.02 Mn0.02 Nd0.02 Bi0.01
Ca0.01 Pb0.01) ((Ta1.75 Nb0.10 Sn0.10 Si0.04 Ti0.01) (O5.77 (O
H)0.23) ((H2 O)0.97) (Cs0.03))
;
_chemical_formula_sum
;
Ba0.33 Bi0.01 Ca0.01 Ce0.02 Cs0.03 H3.13 La0.02 Mn0.02 Nb0.10
Nd0.02 O7.45 Pb0.01 Si0.04 Sn0.10 Sr0.27 Ta1.75 Ti0.01 U0.10
;
_chemical_formula_weight                577.2
_chemical_name_mineral                  unnamed
_chemical_compound_source
;
Minerals from Volta Grande pegmatite, Minas Gerais
;

#------------------ UNIT CELL INFORMATION ------------------------------------#
 _symmetry_cell_setting                 cubic
```

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_symmetry_space_group_name_H-M        'F d -3 m'
_symmetry_space_group_name_Hall    '-F_4vw_2vw_3'
_symmetry_Int_Tables_number            227
loop_
 _symmetry_equiv_pos_as_xyz
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 '-x+3/4, y, -z+3/4'
 '-y, x+1/4, z+1/4'
 'y+3/4, x+1/4, -z+1/2'
 'y+3/4, -x, z+3/4'
 '-y, -x, -z'
 'y, z, x'
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 '-x, z+5/4, y+5/4'
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 'x+3/4, z+3/4, -y+1'
 'x+1/2, y, z+1/2'
 'x+1/2, -y+1/4, -z+3/4'
```

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'y, -x-1/4, -z-1/4'
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'-y, -z, -x'

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'-z-1/4, -y-1/4, x'

```
 '-z+1/2, -x, -y+1/2'
 'z+1/4, -x-1/2, y-1/4'
 'z+1/4, x-1/4, -y+1/2'
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_cell_length_b                    10.4537(12)
_cell_length_c                    10.4537(12)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      1142.4(2)
_cell_formula_units_Z             8
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     331
_cell_measurement_theta_min       3.395
_cell_measurement_theta_max       31.507

#------------------ CRYSTAL INFORMATION ----------------------------------#

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_exptl_crystal_colour                 'pinkish brown'
_exptl_crystal_size_max                0.197
_exptl_crystal_size_mid                0.170
_exptl_crystal_size_min                0.104
_exptl_crystal_density_diffrn          6.7
_exptl_crystal_density_method          'not measured'
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_exptl_crystal_F_000                    1941
_exptl_absorpt_coefficient_mu           38.097
_exptl_absorpt_correction_type          gaussian
_exptl_absorpt_process_details
;
   P. Coppens, L. Leiserowitz, D Rabinovich, Acta Cryst.
   (1965), 18, 1035-1038
;
_exptl_absorpt_correction_T_min         0.012
_exptl_absorpt_correction_T_max         0.072

#------------------ DATA COLLECTION INFORMATION -----------------------------#
_diffrn_ambient_temperature             293(2)
_diffrn_radiation_wavelength            0.71073
_diffrn_radiation_type                  MoK\a
_diffrn_radiation_probe                 x-ray
_diffrn_measurement_device_type         KappaCCD
_diffrn_measurement_device              '95mm CCD camera on \k-goniostat'
_diffrn_measurement_method              '\f scans and \w scans winth \k offsets'
_diffrn_standards_decay_%               0
_diffrn_reflns_number                   319
_diffrn_reflns_av_R_equivalents   0.0559
_diffrn_reflns_av_sigmaI/netI     0.0417
_diffrn_reflns_limit_h_min              -15
_diffrn_reflns_limit_h_max              15
_diffrn_reflns_limit_k_min              -11
_diffrn_reflns_limit_k_max              11
_diffrn_reflns_limit_l_min              -9
_diffrn_reflns_limit_l_max              9
_diffrn_reflns_theta_min                5.52
_diffrn_reflns_theta_max                32.00
_diffrn_reflns_theta_full               32.00
_diffrn_measured_fraction_theta_max     0.992
_diffrn_measured_fraction_theta_full    0.992
_reflns_number_total                    121
_reflns_number_gt                       86
_reflns_threshold_expression            >2\s(I)
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_computing_data_collection              'Collect (Nonius BV, 1997-2000)'
_computing_cell_refinement             'HKL Scalepack (Otwinowski & Minor 1997)'
_computing_data_reduction  'HKL Denzo and Scalepack (Otwinowski & Minor 1997)'
_computing_structure_solution          'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement        'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics          'Ortep-3 for Windows (Farrugia, 1997)'
_computing_publication_material  'WinGX publication routines (Farrugia, 1999)'
#------------------ REFINEMENT INFORMATION ---------------------------------#
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0372P)^2^+70.5641P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    difmap
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_expression
```

```
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_extinction_coef        0.00041(10)
_refine_ls_number_reflns          121
_refine_ls_number_parameters      16
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0620
_refine_ls_R_factor_gt            0.0363
_refine_ls_wR_factor_ref          0.1009
_refine_ls_wR_factor_gt           0.0931
_refine_ls_goodness_of_fit_ref    1.180
_refine_ls_restrained_S_all       1.180
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000
_refine_diff_density_max          1.750
_refine_diff_density_min         -2.165
_refine_diff_density_rms          0.393

#------------------ ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS --------#
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 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Mn'  'Mn'   0.3368   0.7283
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ba'  'Ba'  -0.3244   2.2819
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Sr'  'Sr'  -1.5307   3.2498
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ce'  'Ce'  -0.2486   2.6331
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'U'  'U'  -9.6767   9.6646
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Bi'  'Bi'  -4.1077  10.2566
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Nd'  'Nd'  -0.1943   3.0179
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'La'  'La'  -0.2871   2.4523
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ta'  'Ta'  -0.7052   6.5227
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Nb'  'Nb'  -2.0727   0.6215
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.0817   0.0704
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ti'  'Ti'   0.2776   0.4457
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Sn'  'Sn'  -0.6537   1.4246
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cs'  'Cs'  -0.3680   2.1192
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Pb'  'Pb'  -3.3944  10.1111
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_atom_site_occupancy
_atom_site_U_iso_or_equiv
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Mn Mn 16 d 0.5 0.5 0.5 0.010 0.0556(17)
Ba Ba 16 d 0.5 0.5 0.5 0.165 0.0556(17)
Sr Sr 16 d 0.5 0.5 0.5 0.135 0.0556(17)
Ce Ce 16 d 0.5 0.5 0.5 0.010 0.0556(17)
U  U  16 d 0.5 0.5 0.5 0.050 0.0556(17)
Bi Bi 16 d 0.5 0.5 0.5 0.005 0.0556(17)
Nd Nd 16 d 0.5 0.5 0.5 0.010 0.0556(17)
La La 16 d 0.5 0.5 0.5 0.010 0.0556(17)
Pb Pb 16 d 0.5 0.5 0.5 0.005 0.0556(17)
O1 O  16 d 0.5 0.5 0.5 0.240 0.0556(17)
Ta Ta 16 c 0.0 0.0 0.0 0.875 0.0306(6)
Nb Nb 16 c 0.0 0.0 0.0 0.050 0.0306(6)
Si Si 16 c 0.0 0.0 0.0 0.020 0.0306(6)
Ti Ti 16 c 0.0 0.0 0.0 0.005 0.0306(6)
Sn Sn 16 c 0.0 0.0 0.0 0.050 0.0306(6)
O2 O  48 f 0.3191(14) 0.1250 0.1250 1 0.038(3)
Cs Cs 8  b 0.3750 0.3750 0.3750 0.030 0.051(14)
O4 O  8  b 0.3750 0.3750 0.3750 0.320 0.051(14)
O3 O 32 e 0.748(6) 0.748(6) 0.748(6) 0.16 0.051(14)
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 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.
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Ca Mn Ba 180.0 2_566 26 ?
Ca Mn Ba 60.0 27_554 26 ?
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Ba Mn Ba 180.0 2_566 26 ?
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Ca O4 Sr 0.0 . . ?
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Ba Mn Cs O3 120(100) 26 . . 97_666 ?
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Ca Mn Cs O3 60.000(3) 4 . . 147_556 ?
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O3 Bi Cs O3 -60(100) 98_655 . . 97_666 ?
O3 Bi Cs O3 120(100) 2_566 . . 97_666 ?
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O2 Bi Cs O3 60.000(3) 177_556 . . 98_655 ?
O2 Bi Cs O3 -120.000(3) 81 . . 98_655 ?
O4 Bi Cs Mn 0.0 97_666 . . . ?
O4 Bi Cs Mn 0.0 . . . . ?
Cs Bi Cs Mn 0.0 97_666 . . . ?
O3 Bi Cs Mn 0.0 148_565 . . . ?
O3 Bi Cs Mn 0.0 52 . . . ?
O3 Bi Cs Mn 0.0 147_556 . . . ?
O3 Bi Cs Mn 0.0 51_564 . . . ?
O3 Bi Cs Mn 0.0 98_655 . . . ?
O3 Bi Cs Mn 0.0 2_566 . . . ?
O2 Bi Cs Mn 0.0 177_556 . . . ?
O2 Bi Cs Mn 0.0 81 . . . ?
O4 Bi Cs Ce 0.0 97_666 . . . ?
O4 Bi Cs Ce 0.0 . . . . ?
Cs Bi Cs Ce 0.0 97_666 . . . ?
O3 Bi Cs Ce 0.0 148_565 . . . ?
O3 Bi Cs Ce 0.0 52 . . . ?
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O3 Bi Cs Ce 0.0 147_556 . . . ?
O3 Bi Cs Ce 0.0 51_564 . . . ?
O3 Bi Cs Ce 0.0 98_655 . . . ?
O3 Bi Cs Ce 0.0 2_566 . . . ?
O2 Bi Cs Ce 0.0 177_556 . . . ?
O2 Bi Cs Ce 0.0 81 . . . ?
O4 Bi Cs U 0.0 97_666 . . . ?
O4 Bi Cs U 0.0 . . . . ?
Cs Bi Cs U 0.0 97_666 . . . ?
O3 Bi Cs U 0.0 148_565 . . . ?
O3 Bi Cs U 0.0 52 . . . ?
O3 Bi Cs U 0.0 147_556 . . . ?
O3 Bi Cs U 0.0 51_564 . . . ?
O3 Bi Cs U 0.0 98_655 . . . ?
O3 Bi Cs U 0.0 2_566 . . . ?
O2 Bi Cs U 0.0 177_556 . . . ?
O2 Bi Cs U 0.0 81 . . . ?
O4 Bi Cs Nd 0.0 97_666 . . . ?
O4 Bi Cs Nd 0.0 . . . . ?
Cs Bi Cs Nd 0.0 97_666 . . . ?
O3 Bi Cs Nd 0.0 148_565 . . . ?
O3 Bi Cs Nd 0.0 52 . . . ?
O3 Bi Cs Nd 0.0 147_556 . . . ?
O3 Bi Cs Nd 0.0 51_564 . . . ?
O3 Bi Cs Nd 0.0 98_655 . . . ?
O3 Bi Cs Nd 0.0 2_566 . . . ?
O2 Bi Cs Nd 0.0 177_556 . . . ?
O2 Bi Cs Nd 0.0 81 . . . ?
O4 Bi Cs La 0.0 97_666 . . . ?
O4 Bi Cs La 0.0 . . . . ?
Cs Bi Cs La 0.0 97_666 . . . ?
O3 Bi Cs La 0.0 148_565 . . . ?
O3 Bi Cs La 0.0 52 . . . ?
O3 Bi Cs La 0.0 147_556 . . . ?
O3 Bi Cs La 0.0 51_564 . . . ?
O3 Bi Cs La 0.0 98_655 . . . ?
O3 Bi Cs La 0.0 2_566 . . . ?
O2 Bi Cs La 0.0 177_556 . . . ?
O2 Bi Cs La 0.0 81 . . . ?
O4 Bi Cs Pb 0.0 97_666 . . . ?
O4 Bi Cs Pb 0.0 . . . . ?
Cs Bi Cs Pb 0.0 97_666 . . . ?
O3 Bi Cs Pb 0.0 148_565 . . . ?
O3 Bi Cs Pb 0.0 52 . . . ?
O3 Bi Cs Pb 0.0 147_556 . . . ?
O3 Bi Cs Pb 0.0 51_564 . . . ?
O3 Bi Cs Pb 0.0 98_655 . . . ?
O3 Bi Cs Pb 0.0 2_566 . . . ?
O2 Bi Cs Pb 0.0 177_556 . . . ?
O2 Bi Cs Pb 0.0 81 . . . ?
O4 Bi Cs O1 0.0 97_666 . . . ?
O4 Bi Cs O1 0.0 . . . . ?
Cs Bi Cs O1 0.0 97_666 . . . ?
O3 Bi Cs O1 0.0 148_565 . . . ?
O3 Bi Cs O1 0.0 52 . . . ?
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O3 Bi Cs O1 0.0 147_556 . . . ?
O3 Bi Cs O1 0.0 51_564 . . . ?
O3 Bi Cs O1 0.0 98_655 . . . ?
O3 Bi Cs O1 0.0 2_566 . . . ?
O2 Bi Cs O1 0.0 177_556 . . . ?
O2 Bi Cs O1 0.0 81 . . . ?
O4 Nd Cs O3 0(100) 97_666 . . 97_666 ?
O4 Nd Cs O3 0.0 . . . 97_666 ?
Cs Nd Cs O3 0(100) 97_666 . . 97_666 ?
O3 Nd Cs O3 60(100) 148_565 . . 97_666 ?
O3 Nd Cs O3 -120(100) 52 . . 97_666 ?
O3 Nd Cs O3 -180(100) 147_556 . . 97_666 ?
O3 Nd Cs O3 0(100) 51_564 . . 97_666 ?
O3 Nd Cs O3 -60(100) 98_655 . . 97_666 ?
O3 Nd Cs O3 120(100) 2_566 . . 97_666 ?
O2 Nd Cs O3 0(100) 177_556 . . 97_666 ?
O2 Nd Cs O3 -180(100) 81 . . 97_666 ?
O4 Nd Cs O3 60(100) 97_666 . . 148_565 ?
O4 Nd Cs O3 0.0 . . . 148_565 ?
Cs Nd Cs O3 60(100) 97_666 . . 148_565 ?
O3 Nd Cs O3 180.000(4) 52 . . 148_565 ?
O3 Nd Cs O3 120.000(4) 147_556 . . 148_565 ?
O3 Nd Cs O3 -60.000(5) 51_564 . . 148_565 ?
O3 Nd Cs O3 -120.000(2) 98_655 . . 148_565 ?
O3 Nd Cs O3 60.000(4) 2_566 . . 148_565 ?
O2 Nd Cs O3 -60.000(4) 177_556 . . 148_565 ?
O2 Nd Cs O3 120.000(5) 81 . . 148_565 ?
O4 Nd Cs O3 -60(100) 97_666 . . 147_556 ?
O4 Nd Cs O3 0.0 . . . 147_556 ?
Cs Nd Cs O3 -60(100) 97_666 . . 147_556 ?
O3 Nd Cs O3 -120.000(3) 148_565 . . 147_556 ?
O3 Nd Cs O3 60.0 52 . . 147_556 ?
O3 Nd Cs O3 180.000(4) 51_564 . . 147_556 ?
O3 Nd Cs O3 120.000(3) 98_655 . . 147_556 ?
O3 Nd Cs O3 -60.000(1) 2_566 . . 147_556 ?
O2 Nd Cs O3 180.000(3) 177_556 . . 147_556 ?
O2 Nd Cs O3 0.0 81 . . 147_556 ?
O4 Nd Cs O3 180(100) 97_666 . . 98_655 ?
O4 Nd Cs O3 0.0 . . . 98_655 ?
Cs Nd Cs O3 180(100) 97_666 . . 98_655 ?
O3 Nd Cs O3 120.000(2) 148_565 . . 98_655 ?
O3 Nd Cs O3 -60.000(4) 52 . . 98_655 ?
O3 Nd Cs O3 -120.000(4) 147_556 . . 98_655 ?
O3 Nd Cs O3 60.000(1) 51_564 . . 98_655 ?
O3 Nd Cs O3 180.000(3) 2_566 . . 98_655 ?
O2 Nd Cs O3 60.000(3) 177_556 . . 98_655 ?
O2 Nd Cs O3 -120.000(3) 81 . . 98_655 ?
O4 Nd Cs Mn 0.0 97_666 . . . ?
O4 Nd Cs Mn 0.0 . . . . ?
Cs Nd Cs Mn 0.0 97_666 . . . ?
O3 Nd Cs Mn 0.0 148_565 . . . ?
O3 Nd Cs Mn 0.0 52 . . . ?
O3 Nd Cs Mn 0.0 147_556 . . . ?
O3 Nd Cs Mn 0.0 51_564 . . . ?
O3 Nd Cs Mn 0.0 98_655 . . . ?
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O3 Nd Cs Mn 0.0 2_566 . . . ?
O2 Nd Cs Mn 0.0 177_556 . . . ?
O2 Nd Cs Mn 0.0 81 . . . ?
O4 Nd Cs Ce 0.0 97_666 . . . ?
O4 Nd Cs Ce 0.0 . . . . ?
Cs Nd Cs Ce 0.0 97_666 . . . ?
O3 Nd Cs Ce 0.0 148_565 . . . ?
O3 Nd Cs Ce 0.0 52 . . . ?
O3 Nd Cs Ce 0.0 147_556 . . . ?
O3 Nd Cs Ce 0.0 51_564 . . . ?
O3 Nd Cs Ce 0.0 98_655 . . . ?
O3 Nd Cs Ce 0.0 2_566 . . . ?
O2 Nd Cs Ce 0.0 177_556 . . . ?
O2 Nd Cs Ce 0.0 81 . . . ?
O4 Nd Cs U 0.0 97_666 . . . ?
O4 Nd Cs U 0.0 . . . . ?
Cs Nd Cs U 0.0 97_666 . . . ?
O3 Nd Cs U 0.0 148_565 . . . ?
O3 Nd Cs U 0.0 52 . . . ?
O3 Nd Cs U 0.0 147_556 . . . ?
O3 Nd Cs U 0.0 51_564 . . . ?
O3 Nd Cs U 0.0 98_655 . . . ?
O3 Nd Cs U 0.0 2_566 . . . ?
O2 Nd Cs U 0.0 177_556 . . . ?
O2 Nd Cs U 0.0 81 . . . ?
O4 Nd Cs Bi 0.0 97_666 . . . ?
O4 Nd Cs Bi 0.0 . . . . ?
Cs Nd Cs Bi 0.0 97_666 . . . ?
O3 Nd Cs Bi 0.0 148_565 . . . ?
O3 Nd Cs Bi 0.0 52 . . . ?
O3 Nd Cs Bi 0.0 147_556 . . . ?
O3 Nd Cs Bi 0.0 51_564 . . . ?
O3 Nd Cs Bi 0.0 98_655 . . . ?
O3 Nd Cs Bi 0.0 2_566 . . . ?
O2 Nd Cs Bi 0.0 177_556 . . . ?
O2 Nd Cs Bi 0.0 81 . . . ?
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O4 Nd Cs La 0.0 . . . . ?
Cs Nd Cs La 0.0 97_666 . . . ?
O3 Nd Cs La 0.0 148_565 . . . ?
O3 Nd Cs La 0.0 52 . . . ?
O3 Nd Cs La 0.0 147_556 . . . ?
O3 Nd Cs La 0.0 51_564 . . . ?
O3 Nd Cs La 0.0 98_655 . . . ?
O3 Nd Cs La 0.0 2_566 . . . ?
O2 Nd Cs La 0.0 177_556 . . . ?
O2 Nd Cs La 0.0 81 . . . ?
O4 Nd Cs Pb 0.0 97_666 . . . ?
O4 Nd Cs Pb 0.0 . . . . ?
Cs Nd Cs Pb 0.0 97_666 . . . ?
O3 Nd Cs Pb 0.0 148_565 . . . ?
O3 Nd Cs Pb 0.0 52 . . . ?
O3 Nd Cs Pb 0.0 147_556 . . . ?
O3 Nd Cs Pb 0.0 51_564 . . . ?
O3 Nd Cs Pb 0.0 98_655 . . . ?
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O2 Nd Cs Pb 0.0 177_556 . . . ?
O2 Nd Cs Pb 0.0 81 . . . ?
O4 Nd Cs O1 0.0 97_666 . . . ?
O4 Nd Cs O1 0.0 . . . . ?
Cs Nd Cs O1 0.0 97_666 . . . ?
O3 Nd Cs O1 0.0 148_565 . . . ?
O3 Nd Cs O1 0.0 52 . . . ?
O3 Nd Cs O1 0.0 147_556 . . . ?
O3 Nd Cs O1 0.0 51_564 . . . ?
O3 Nd Cs O1 0.0 98_655 . . . ?
O3 Nd Cs O1 0.0 2_566 . . . ?
O2 Nd Cs O1 0.0 177_556 . . . ?
O2 Nd Cs O1 0.0 81 . . . ?
O4 La Cs O3 0(100) 97_666 . . 97_666 ?
O4 La Cs O3 0.0 . . . 97_666 ?
Cs La Cs O3 0(100) 97_666 . . 97_666 ?
O3 La Cs O3 60(100) 148_565 . . 97_666 ?
O3 La Cs O3 -120(100) 52 . . 97_666 ?
O3 La Cs O3 -180(100) 147_556 . . 97_666 ?
O3 La Cs O3 0(100) 51_564 . . 97_666 ?
O3 La Cs O3 -60(100) 98_655 . . 97_666 ?
O3 La Cs O3 120(100) 2_566 . . 97_666 ?
O2 La Cs O3 0(100) 177_556 . . 97_666 ?
O2 La Cs O3 -180(100) 81 . . 97_666 ?
O4 La Cs O3 60(100) 97_666 . . 148_565 ?
O4 La Cs O3 0.0 . . . 148_565 ?
Cs La Cs O3 60(100) 97_666 . . 148_565 ?
O3 La Cs O3 180.000(4) 52 . . 148_565 ?
O3 La Cs O3 120.000(4) 147_556 . . 148_565 ?
O3 La Cs O3 -60.000(5) 51_564 . . 148_565 ?
O3 La Cs O3 -120.000(2) 98_655 . . 148_565 ?
O3 La Cs O3 60.000(4) 2_566 . . 148_565 ?
O2 La Cs O3 -60.000(4) 177_556 . . 148_565 ?
O2 La Cs O3 120.000(5) 81 . . 148_565 ?
O4 La Cs O3 -60(100) 97_666 . . 147_556 ?
O4 La Cs O3 0.0 . . . 147_556 ?
Cs La Cs O3 -60(100) 97_666 . . 147_556 ?
O3 La Cs O3 -120.000(3) 148_565 . . 147_556 ?
O3 La Cs O3 60.0 52 . . 147_556 ?
O3 La Cs O3 180.000(4) 51_564 . . 147_556 ?
O3 La Cs O3 120.000(3) 98_655 . . 147_556 ?
O3 La Cs O3 -60.000(1) 2_566 . . 147_556 ?
O2 La Cs O3 180.000(3) 177_556 . . 147_556 ?
O2 La Cs O3 0.0 81 . . 147_556 ?
O4 La Cs O3 180(100) 97_666 . . 98_655 ?
O4 La Cs O3 0.0 . . . 98_655 ?
Cs La Cs O3 180(100) 97_666 . . 98_655 ?
O3 La Cs O3 120.000(2) 148_565 . . 98_655 ?
O3 La Cs O3 -60.000(4) 52 . . 98_655 ?
O3 La Cs O3 -120.000(4) 147_556 . . 98_655 ?
O3 La Cs O3 60.000(1) 51_564 . . 98_655 ?
O3 La Cs O3 180.000(3) 2_566 . . 98_655 ?
O2 La Cs O3 60.000(3) 177_556 . . 98_655 ?
O2 La Cs O3 -120.000(3) 81 . . 98_655 ?
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O4 La Cs Mn 0.0 . . . . ?
Cs La Cs Mn 0.0 97_666 . . . ?
O3 La Cs Mn 0.0 148_565 . . . ?
O3 La Cs Mn 0.0 52 . . . ?
O3 La Cs Mn 0.0 147_556 . . . ?
O3 La Cs Mn 0.0 51_564 . . . ?
O3 La Cs Mn 0.0 98_655 . . . ?
O3 La Cs Mn 0.0 2_566 . . . ?
O2 La Cs Mn 0.0 177_556 . . . ?
O2 La Cs Mn 0.0 81 . . . ?
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O4 La Cs Ce 0.0 . . . . ?
Cs La Cs Ce 0.0 97_666 . . . ?
O3 La Cs Ce 0.0 148_565 . . . ?
O3 La Cs Ce 0.0 52 . . . ?
O3 La Cs Ce 0.0 147_556 . . . ?
O3 La Cs Ce 0.0 51_564 . . . ?
O3 La Cs Ce 0.0 98_655 . . . ?
O3 La Cs Ce 0.0 2_566 . . . ?
O2 La Cs Ce 0.0 177_556 . . . ?
O2 La Cs Ce 0.0 81 . . . ?
O4 La Cs U 0.0 97_666 . . . ?
O4 La Cs U 0.0 . . . . ?
Cs La Cs U 0.0 97_666 . . . ?
O3 La Cs U 0.0 148_565 . . . ?
O3 La Cs U 0.0 52 . . . ?
O3 La Cs U 0.0 147_556 . . . ?
O3 La Cs U 0.0 51_564 . . . ?
O3 La Cs U 0.0 98_655 . . . ?
O3 La Cs U 0.0 2_566 . . . ?
O2 La Cs U 0.0 177_556 . . . ?
O2 La Cs U 0.0 81 . . . ?
O4 La Cs Bi 0.0 97_666 . . . ?
O4 La Cs Bi 0.0 . . . . ?
Cs La Cs Bi 0.0 97_666 . . . ?
O3 La Cs Bi 0.0 148_565 . . . ?
O3 La Cs Bi 0.0 52 . . . ?
O3 La Cs Bi 0.0 147_556 . . . ?
O3 La Cs Bi 0.0 51_564 . . . ?
O3 La Cs Bi 0.0 98_655 . . . ?
O3 La Cs Bi 0.0 2_566 . . . ?
O2 La Cs Bi 0.0 177_556 . . . ?
O2 La Cs Bi 0.0 81 . . . ?
O4 La Cs Nd 0.0 97_666 . . . ?
O4 La Cs Nd 0.0 . . . . ?
Cs La Cs Nd 0.0 97_666 . . . ?
O3 La Cs Nd 0.0 148_565 . . . ?
O3 La Cs Nd 0.0 52 . . . ?
O3 La Cs Nd 0.0 147_556 . . . ?
O3 La Cs Nd 0.0 51_564 . . . ?
O3 La Cs Nd 0.0 98_655 . . . ?
O3 La Cs Nd 0.0 2_566 . . . ?
O2 La Cs Nd 0.0 177_556 . . . ?
O2 La Cs Nd 0.0 81 . . . ?
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O4 La Cs Pb 0.0 97_666 . . . ?
O4 La Cs Pb 0.0 . . . . ?
Cs La Cs Pb 0.0 97_666 . . . ?
O3 La Cs Pb 0.0 148_565 . . . ?
O3 La Cs Pb 0.0 52 . . . ?
O3 La Cs Pb 0.0 147_556 . . . ?
O3 La Cs Pb 0.0 51_564 . . . ?
O3 La Cs Pb 0.0 98_655 . . . ?
O3 La Cs Pb 0.0 2_566 . . . ?
O2 La Cs Pb 0.0 177_556 . . . ?
O2 La Cs Pb 0.0 81 . . . ?
O4 La Cs O1 0.0 97_666 . . . ?
O4 La Cs O1 0.0 . . . . ?
Cs La Cs O1 0.0 97_666 . . . ?
O3 La Cs O1 0.0 148_565 . . . ?
O3 La Cs O1 0.0 52 . . . ?
O3 La Cs O1 0.0 147_556 . . . ?
O3 La Cs O1 0.0 51_564 . . . ?
O3 La Cs O1 0.0 98_655 . . . ?
O3 La Cs O1 0.0 2_566 . . . ?
O2 La Cs O1 0.0 177_556 . . . ?
O2 La Cs O1 0.0 81 . . . ?
O4 Pb Cs O3 0(100) 97_666 . . 97_666 ?
O4 Pb Cs O3 0.0 . . . 97_666 ?
Cs Pb Cs O3 0(100) 97_666 . . 97_666 ?
O3 Pb Cs O3 60(100) 148_565 . . 97_666 ?
O3 Pb Cs O3 -120(100) 52 . . 97_666 ?
O3 Pb Cs O3 -180(100) 147_556 . . 97_666 ?
O3 Pb Cs O3 0(100) 51_564 . . 97_666 ?
O3 Pb Cs O3 -60(100) 98_655 . . 97_666 ?
O3 Pb Cs O3 120(100) 2_566 . . 97_666 ?
O2 Pb Cs O3 0(100) 177_556 . . 97_666 ?
O2 Pb Cs O3 -180(100) 81 . . 97_666 ?
O4 Pb Cs O3 60(100) 97_666 . . 148_565 ?
O4 Pb Cs O3 0.0 . . . 148_565 ?
Cs Pb Cs O3 60(100) 97_666 . . 148_565 ?
O3 Pb Cs O3 180.000(4) 52 . . 148_565 ?
O3 Pb Cs O3 120.000(4) 147_556 . . 148_565 ?
O3 Pb Cs O3 -60.000(5) 51_564 . . 148_565 ?
O3 Pb Cs O3 -120.000(2) 98_655 . . 148_565 ?
O3 Pb Cs O3 60.000(4) 2_566 . . 148_565 ?
O2 Pb Cs O3 -60.000(4) 177_556 . . 148_565 ?
O2 Pb Cs O3 120.000(5) 81 . . 148_565 ?
O4 Pb Cs O3 -60(100) 97_666 . . 147_556 ?
O4 Pb Cs O3 0.0 . . . 147_556 ?
Cs Pb Cs O3 -60(100) 97_666 . . 147_556 ?
O3 Pb Cs O3 -120.000(3) 148_565 . . 147_556 ?
O3 Pb Cs O3 60.0 52 . . 147_556 ?
O3 Pb Cs O3 180.000(4) 51_564 . . 147_556 ?
O3 Pb Cs O3 120.000(3) 98_655 . . 147_556 ?
O3 Pb Cs O3 -60.000(1) 2_566 . . 147_556 ?
O2 Pb Cs O3 180.000(3) 177_556 . . 147_556 ?
O2 Pb Cs O3 0.0 81 . . 147_556 ?
O4 Pb Cs O3 180(100) 97_666 . . 98_655 ?
O4 Pb Cs O3 0.0 . . . 98_655 ?
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Cs Pb Cs O3 180(100) 97_666 . . 98_655 ?
O3 Pb Cs O3 120.000(2) 148_565 . . 98_655 ?
O3 Pb Cs O3 -60.000(4) 52 . . 98_655 ?
O3 Pb Cs O3 -120.000(4) 147_556 . . 98_655 ?
O3 Pb Cs O3 60.000(1) 51_564 . . 98_655 ?
O3 Pb Cs O3 180.000(3) 2_566 . . 98_655 ?
O2 Pb Cs O3 60.000(3) 177_556 . . 98_655 ?
O2 Pb Cs O3 -120.000(3) 81 . . 98_655 ?
O4 Pb Cs Mn 0.0 97_666 . . . ?
O4 Pb Cs Mn 0.0 . . . . ?
Cs Pb Cs Mn 0.0 97_666 . . . ?
O3 Pb Cs Mn 0.0 148_565 . . . ?
O3 Pb Cs Mn 0.0 52 . . . ?
O3 Pb Cs Mn 0.0 147_556 . . . ?
O3 Pb Cs Mn 0.0 51_564 . . . ?
O3 Pb Cs Mn 0.0 98_655 . . . ?
O3 Pb Cs Mn 0.0 2_566 . . . ?
O2 Pb Cs Mn 0.0 177_556 . . . ?
O2 Pb Cs Mn 0.0 81 . . . ?
O4 Pb Cs Ce 0.0 97_666 . . . ?
O4 Pb Cs Ce 0.0 . . . . ?
Cs Pb Cs Ce 0.0 97_666 . . . ?
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O3 Pb Cs Ce 0.0 52 . . . ?
O3 Pb Cs Ce 0.0 147_556 . . . ?
O3 Pb Cs Ce 0.0 51_564 . . . ?
O3 Pb Cs Ce 0.0 98_655 . . . ?
O3 Pb Cs Ce 0.0 2_566 . . . ?
O2 Pb Cs Ce 0.0 177_556 . . . ?
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O3 Pb Cs U 0.0 52 . . . ?
O3 Pb Cs U 0.0 147_556 . . . ?
O3 Pb Cs U 0.0 51_564 . . . ?
O3 Pb Cs U 0.0 98_655 . . . ?
O3 Pb Cs U 0.0 2_566 . . . ?
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O2 Pb Cs U 0.0 81 . . . ?
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O4 Pb Cs Bi 0.0 . . . . ?
Cs Pb Cs Bi 0.0 97_666 . . . ?
O3 Pb Cs Bi 0.0 148_565 . . . ?
O3 Pb Cs Bi 0.0 52 . . . ?
O3 Pb Cs Bi 0.0 147_556 . . . ?
O3 Pb Cs Bi 0.0 51_564 . . . ?
O3 Pb Cs Bi 0.0 98_655 . . . ?
O3 Pb Cs Bi 0.0 2_566 . . . ?
O2 Pb Cs Bi 0.0 177_556 . . . ?
O2 Pb Cs Bi 0.0 81 . . . ?
O4 Pb Cs Nd 0.0 97_666 . . . ?
O4 Pb Cs Nd 0.0 . . . . ?
Cs Pb Cs Nd 0.0 97_666 . . . ?
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O3 Pb Cs Nd 0.0 52 . . . ?
O3 Pb Cs Nd 0.0 147_556 . . . ?
O3 Pb Cs Nd 0.0 51_564 . . . ?
O3 Pb Cs Nd 0.0 98_655 . . . ?
O3 Pb Cs Nd 0.0 2_566 . . . ?
O2 Pb Cs Nd 0.0 177_556 . . . ?
O2 Pb Cs Nd 0.0 81 . . . ?
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O4 Pb Cs La 0.0 . . . . ?
Cs Pb Cs La 0.0 97_666 . . . ?
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O3 Pb Cs La 0.0 52 . . . ?
O3 Pb Cs La 0.0 147_556 . . . ?
O3 Pb Cs La 0.0 51_564 . . . ?
O3 Pb Cs La 0.0 98_655 . . . ?
O3 Pb Cs La 0.0 2_566 . . . ?
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O2 Pb Cs La 0.0 81 . . . ?
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O4 Pb Cs O1 0.0 . . . . ?
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O3 Pb Cs O1 0.0 52 . . . ?
O3 Pb Cs O1 0.0 147_556 . . . ?
O3 Pb Cs O1 0.0 51_564 . . . ?
O3 Pb Cs O1 0.0 98_655 . . . ?
O3 Pb Cs O1 0.0 2_566 . . . ?
O2 Pb Cs O1 0.0 177_556 . . . ?
O2 Pb Cs O1 0.0 81 . . . ?
Cs O1 Cs O3 0(100) 97_666 . . 97_666 ?
Cs O1 Cs O3 60(100) 97_666 . . 148_565 ?
Cs O1 Cs O3 -60(100) 97_666 . . 147_556 ?
Cs O1 Cs O3 180(100) 97_666 . . 98_655 ?
Cs O1 Cs Mn 0.0 97_666 . . . ?
Cs O1 Cs Ce 0.0 97_666 . . . ?
Cs O1 Cs U 0.0 97_666 . . . ?
Cs O1 Cs Bi 0.0 97_666 . . . ?
Cs O1 Cs Nd 0.0 97_666 . . . ?
Cs O1 Cs La 0.0 97_666 . . . ?
Cs O1 Cs Pb 0.0 97_666 . . . ?
O4 Pb O4 Ca 0.0 97_666 . . . ?
Cs Pb O4 Ca 0.0 . . . . ?
Cs Pb O4 Ca 0.0 97_666 . . . ?
O3 Pb O4 Ca 0.0 148_565 . . . ?
O3 Pb O4 Ca 0.0 52 . . . ?
O3 Pb O4 Ca 0.0 147_556 . . . ?
O3 Pb O4 Ca 0.0 51_564 . . . ?
O3 Pb O4 Ca 0.0 98_655 . . . ?
O3 Pb O4 Ca 0.0 2_566 . . . ?
O2 Pb O4 Ca 0.0 177_556 . . . ?
O2 Pb O4 Ca 0.0 81 . . . ?
O4 Pb O4 Mn 0.0 97_666 . . . ?
Cs Pb O4 Mn 0.0 . . . . ?
Cs Pb O4 Mn 0.0 97_666 . . . ?
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```
O3 Pb O4 Mn 0.0 148_565 . . . ?
O3 Pb O4 Mn 0.0 52 . . . ?
O3 Pb O4 Mn 0.0 147_556 . . . ?
O3 Pb O4 Mn 0.0 51_564 . . . ?
O3 Pb O4 Mn 0.0 98_655 . . . ?
O3 Pb O4 Mn 0.0 2_566 . . . ?
O2 Pb O4 Mn 0.0 177_556 . . . ?
O2 Pb O4 Mn 0.0 81 . . . ?
O4 Pb O4 Ba 0.0 97_666 . . . ?
Cs Pb O4 Ba 0.0 . . . . ?
Cs Pb O4 Ba 0.0 97_666 . . . ?
O3 Pb O4 Ba 0.0 148_565 . . . ?
O3 Pb O4 Ba 0.0 52 . . . ?
O3 Pb O4 Ba 0.0 147_556 . . . ?
O3 Pb O4 Ba 0.0 51_564 . . . ?
O3 Pb O4 Ba 0.0 98_655 . . . ?
O3 Pb O4 Ba 0.0 2_566 . . . ?
O2 Pb O4 Ba 0.0 177_556 . . . ?
O2 Pb O4 Ba 0.0 81 . . . ?
O4 Pb O4 Sr 0.0 97_666 . . . ?
Cs Pb O4 Sr 0.0 . . . . ?
Cs Pb O4 Sr 0.0 97_666 . . . ?
O3 Pb O4 Sr 0.0 148_565 . . . ?
O3 Pb O4 Sr 0.0 52 . . . ?
O3 Pb O4 Sr 0.0 147_556 . . . ?
O3 Pb O4 Sr 0.0 51_564 . . . ?
O3 Pb O4 Sr 0.0 98_655 . . . ?
O3 Pb O4 Sr 0.0 2_566 . . . ?
O2 Pb O4 Sr 0.0 177_556 . . . ?
O2 Pb O4 Sr 0.0 81 . . . ?
O4 Pb O4 Ce 0.0 97_666 . . . ?
Cs Pb O4 Ce 0.0 . . . . ?
Cs Pb O4 Ce 0.0 97_666 . . . ?
O3 Pb O4 Ce 0.0 148_565 . . . ?
O3 Pb O4 Ce 0.0 52 . . . ?
O3 Pb O4 Ce 0.0 147_556 . . . ?
O3 Pb O4 Ce 0.0 51_564 . . . ?
O3 Pb O4 Ce 0.0 98_655 . . . ?
O3 Pb O4 Ce 0.0 2_566 . . . ?
O2 Pb O4 Ce 0.0 177_556 . . . ?
O2 Pb O4 Ce 0.0 81 . . . ?
O4 Pb O4 U 0.0 97_666 . . . ?
Cs Pb O4 U 0.0 . . . . ?
Cs Pb O4 U 0.0 97_666 . . . ?
O3 Pb O4 U 0.0 148_565 . . . ?
O3 Pb O4 U 0.0 52 . . . ?
O3 Pb O4 U 0.0 147_556 . . . ?
O3 Pb O4 U 0.0 51_564 . . . ?
O3 Pb O4 U 0.0 98_655 . . . ?
O3 Pb O4 U 0.0 2_566 . . . ?
O2 Pb O4 U 0.0 177_556 . . . ?
O2 Pb O4 U 0.0 81 . . . ?
O4 Pb O4 Bi 0.0 97_666 . . . ?
Cs Pb O4 Bi 0.0 . . . . ?
Cs Pb O4 Bi 0.0 97_666 . . . ?
```

```
O3 Pb O4 Bi 0.0 148_565 . . . ?
O3 Pb O4 Bi 0.0 52 . . . ?
O3 Pb O4 Bi 0.0 147_556 . . . ?
O3 Pb O4 Bi 0.0 51_564 . . . ?
O3 Pb O4 Bi 0.0 98_655 . . . ?
O3 Pb O4 Bi 0.0 2_566 . . . ?
O2 Pb O4 Bi 0.0 177_556 . . . ?
O2 Pb O4 Bi 0.0 81 . . . ?
O4 Pb O4 Nd 0.0 97_666 . . . ?
Cs Pb O4 Nd 0.0 . . . . ?
Cs Pb O4 Nd 0.0 97_666 . . . ?
O3 Pb O4 Nd 0.0 148_565 . . . ?
O3 Pb O4 Nd 0.0 52 . . . ?
O3 Pb O4 Nd 0.0 147_556 . . . ?
O3 Pb O4 Nd 0.0 51_564 . . . ?
O3 Pb O4 Nd 0.0 98_655 . . . ?
O3 Pb O4 Nd 0.0 2_566 . . . ?
O2 Pb O4 Nd 0.0 177_556 . . . ?
O2 Pb O4 Nd 0.0 81 . . . ?
O4 Pb O4 La 0.0 97_666 . . . ?
Cs Pb O4 La 0.0 . . . . ?
Cs Pb O4 La 0.0 97_666 . . . ?
O3 Pb O4 La 0.0 148_565 . . . ?
O3 Pb O4 La 0.0 52 . . . ?
O3 Pb O4 La 0.0 147_556 . . . ?
O3 Pb O4 La 0.0 51_564 . . . ?
O3 Pb O4 La 0.0 98_655 . . . ?
O3 Pb O4 La 0.0 2_566 . . . ?
O2 Pb O4 La 0.0 177_556 . . . ?
O2 Pb O4 La 0.0 81 . . . ?
O4 Pb O4 Pb -120(100) 97_666 . . 4 ?
Cs Pb O4 Pb 0.0 . . . 4 ?
Cs Pb O4 Pb -120(100) 97_666 . . 4 ?
O3 Pb O4 Pb 180.0 148_565 . . 4 ?
O3 Pb O4 Pb 0.0 52 . . 4 ?
O3 Pb O4 Pb -60.0 147_556 . . 4 ?
O3 Pb O4 Pb 120.0 51_564 . . 4 ?
O3 Pb O4 Pb 60.0 98_655 . . 4 ?
O3 Pb O4 Pb -120.0 2_566 . . 4 ?
O2 Pb O4 Pb 120.0 177_556 . . 4 ?
O2 Pb O4 Pb -60.0 81 . . 4 ?
O4 Pb O4 Ca 0(100) 97_666 . . 26 ?
Cs Pb O4 Ca 0.0 . . . 26 ?
Cs Pb O4 Ca 0(100) 97_666 . . 26 ?
O3 Pb O4 Ca -60.0 148_565 . . 26 ?
O3 Pb O4 Ca 120.0 52 . . 26 ?
O3 Pb O4 Ca 60.0 147_556 . . 26 ?
O3 Pb O4 Ca -120.0 51_564 . . 26 ?
O3 Pb O4 Ca 180.0 98_655 . . 26 ?
O3 Pb O4 Ca 0.0 2_566 . . 26 ?
O2 Pb O4 Ca -120.0 177_556 . . 26 ?
O2 Pb O4 Ca 60.0 81 . . 26 ?
O4 Ca O4 Pb 0.0 97_666 . . . ?
Cs Ca O4 Pb 0.0 . . . . ?
Cs Ca O4 Pb 0.0 97_666 . . . ?
```

```
O3 Ca O4 Pb 0.0 148_565 . . . ?
O3 Ca O4 Pb 0.0 52 . . . ?
O3 Ca O4 Pb 0.0 147_556 . . . ?
O3 Ca O4 Pb 0.0 51_564 . . . ?
O3 Ca O4 Pb 0.0 98_655 . . . ?
O3 Ca O4 Pb 0.0 2_566 . . . ?
O2 Ca O4 Pb 0.0 177_556 . . . ?
O2 Ca O4 Pb 0.0 81 . . . ?
O4 Ca O4 Mn 0.0 97_666 . . . ?
Cs Ca O4 Mn 0.0 . . . . ?
Cs Ca O4 Mn 0.0 97_666 . . . ?
O3 Ca O4 Mn 0.0 148_565 . . . ?
O3 Ca O4 Mn 0.0 52 . . . ?
O3 Ca O4 Mn 0.0 147_556 . . . ?
O3 Ca O4 Mn 0.0 51_564 . . . ?
O3 Ca O4 Mn 0.0 98_655 . . . ?
O3 Ca O4 Mn 0.0 2_566 . . . ?
O2 Ca O4 Mn 0.0 177_556 . . . ?
O2 Ca O4 Mn 0.0 81 . . . ?
O4 Ca O4 Ba 0.0 97_666 . . . ?
Cs Ca O4 Ba 0.0 . . . . ?
Cs Ca O4 Ba 0.0 97_666 . . . ?
O3 Ca O4 Ba 0.0 148_565 . . . ?
O3 Ca O4 Ba 0.0 52 . . . ?
O3 Ca O4 Ba 0.0 147_556 . . . ?
O3 Ca O4 Ba 0.0 51_564 . . . ?
O3 Ca O4 Ba 0.0 98_655 . . . ?
O3 Ca O4 Ba 0.0 2_566 . . . ?
O2 Ca O4 Ba 0.0 177_556 . . . ?
O2 Ca O4 Ba 0.0 81 . . . ?
O4 Ca O4 Sr 0.0 97_666 . . . ?
Cs Ca O4 Sr 0.0 . . . . ?
Cs Ca O4 Sr 0.0 97_666 . . . ?
O3 Ca O4 Sr 0.0 148_565 . . . ?
O3 Ca O4 Sr 0.0 52 . . . ?
O3 Ca O4 Sr 0.0 147_556 . . . ?
O3 Ca O4 Sr 0.0 51_564 . . . ?
O3 Ca O4 Sr 0.0 98_655 . . . ?
O3 Ca O4 Sr 0.0 2_566 . . . ?
O2 Ca O4 Sr 0.0 177_556 . . . ?
O2 Ca O4 Sr 0.0 81 . . . ?
O4 Ca O4 Ce 0.0 97_666 . . . ?
Cs Ca O4 Ce 0.0 . . . . ?
Cs Ca O4 Ce 0.0 97_666 . . . ?
O3 Ca O4 Ce 0.0 148_565 . . . ?
O3 Ca O4 Ce 0.0 52 . . . ?
O3 Ca O4 Ce 0.0 147_556 . . . ?
O3 Ca O4 Ce 0.0 51_564 . . . ?
O3 Ca O4 Ce 0.0 98_655 . . . ?
O3 Ca O4 Ce 0.0 2_566 . . . ?
O2 Ca O4 Ce 0.0 177_556 . . . ?
O2 Ca O4 Ce 0.0 81 . . . ?
O4 Ca O4 U 0.0 97_666 . . . ?
Cs Ca O4 U 0.0 . . . . ?
Cs Ca O4 U 0.0 97_666 . . . ?
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```
O3 Ca O4 U 0.0 148_565 . . . ?
O3 Ca O4 U 0.0 52 . . . ?
O3 Ca O4 U 0.0 147_556 . . . ?
O3 Ca O4 U 0.0 51_564 . . . ?
O3 Ca O4 U 0.0 98_655 . . . ?
O3 Ca O4 U 0.0 2_566 . . . ?
O2 Ca O4 U 0.0 177_556 . . . ?
O2 Ca O4 U 0.0 81 . . . ?
O4 Ca O4 Bi 0.0 97_666 . . . ?
Cs Ca O4 Bi 0.0 . . . . ?
Cs Ca O4 Bi 0.0 97_666 . . . ?
O3 Ca O4 Bi 0.0 148_565 . . . ?
O3 Ca O4 Bi 0.0 52 . . . ?
O3 Ca O4 Bi 0.0 147_556 . . . ?
O3 Ca O4 Bi 0.0 51_564 . . . ?
O3 Ca O4 Bi 0.0 98_655 . . . ?
O3 Ca O4 Bi 0.0 2_566 . . . ?
O2 Ca O4 Bi 0.0 177_556 . . . ?
O2 Ca O4 Bi 0.0 81 . . . ?
O4 Ca O4 Nd 0.0 97_666 . . . ?
Cs Ca O4 Nd 0.0 . . . . ?
Cs Ca O4 Nd 0.0 97_666 . . . ?
O3 Ca O4 Nd 0.0 148_565 . . . ?
O3 Ca O4 Nd 0.0 52 . . . ?
O3 Ca O4 Nd 0.0 147_556 . . . ?
O3 Ca O4 Nd 0.0 51_564 . . . ?
O3 Ca O4 Nd 0.0 98_655 . . . ?
O3 Ca O4 Nd 0.0 2_566 . . . ?
O2 Ca O4 Nd 0.0 177_556 . . . ?
O2 Ca O4 Nd 0.0 81 . . . ?
O4 Ca O4 La 0.0 97_666 . . . ?
Cs Ca O4 La 0.0 . . . . ?
Cs Ca O4 La 0.0 97_666 . . . ?
O3 Ca O4 La 0.0 148_565 . . . ?
O3 Ca O4 La 0.0 52 . . . ?
O3 Ca O4 La 0.0 147_556 . . . ?
O3 Ca O4 La 0.0 51_564 . . . ?
O3 Ca O4 La 0.0 98_655 . . . ?
O3 Ca O4 La 0.0 2_566 . . . ?
O2 Ca O4 La 0.0 177_556 . . . ?
O2 Ca O4 La 0.0 81 . . . ?
O4 Ca O4 Pb -120(100) 97_666 . . 4 ?
Cs Ca O4 Pb 0.0 . . . 4 ?
Cs Ca O4 Pb -120(100) 97_666 . . 4 ?
O3 Ca O4 Pb 180.0 148_565 . . 4 ?
O3 Ca O4 Pb 0.0 52 . . 4 ?
O3 Ca O4 Pb -60.0 147_556 . . 4 ?
O3 Ca O4 Pb 120.0 51_564 . . 4 ?
O3 Ca O4 Pb 60.0 98_655 . . 4 ?
O3 Ca O4 Pb -120.0 2_566 . . 4 ?
O2 Ca O4 Pb 120.0 177_556 . . 4 ?
O2 Ca O4 Pb -60.0 81 . . 4 ?
O4 Ca O4 Ca 0(100) 97_666 . . 26 ?
Cs Ca O4 Ca 0.0 . . . 26 ?
Cs Ca O4 Ca 0(100) 97_666 . . 26 ?
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```
O3 Ca O4 Ca -60.0 148_565 . . 26 ?
O3 Ca O4 Ca 120.0 52 . . 26 ?
O3 Ca O4 Ca 60.0 147_556 . . 26 ?
O3 Ca O4 Ca -120.0 51_564 . . 26 ?
O3 Ca O4 Ca 180.0 98_655 . . 26 ?
O3 Ca O4 Ca 0.0 2_566 . . 26 ?
O2 Ca O4 Ca -120.0 177_556 . . 26 ?
O2 Ca O4 Ca 60.0 81 . . 26 ?
O4 Mn O4 Pb 0.0 97_666 . . . ?
Cs Mn O4 Pb 0.0 . . . . ?
Cs Mn O4 Pb 0.0 97_666 . . . ?
Ca Mn O4 Pb 0.0 2_566 . . . ?
Ca Mn O4 Pb 0.0 27_554 . . . ?
Ca Mn O4 Pb 0.0 51_564 . . . ?
Ca Mn O4 Pb 0.0 4 . . . ?
Ca Mn O4 Pb 0.0 52 . . . ?
Ba Mn O4 Pb 0.0 2_566 . . . ?
Ba Mn O4 Pb 0.0 26 . . . ?
Ba Mn O4 Pb 0.0 27_554 . . . ?
O4 Mn O4 Ca 0.0 97_666 . . . ?
Cs Mn O4 Ca 0.0 . . . . ?
Cs Mn O4 Ca 0.0 97_666 . . . ?
Ca Mn O4 Ca 0.0 2_566 . . . ?
Ca Mn O4 Ca 0.0 27_554 . . . ?
Ca Mn O4 Ca 0.0 51_564 . . . ?
Ca Mn O4 Ca 0.0 4 . . . ?
Ca Mn O4 Ca 0.0 52 . . . ?
Ba Mn O4 Ca 0.0 2_566 . . . ?
Ba Mn O4 Ca 0.0 26 . . . ?
Ba Mn O4 Ca 0.0 27_554 . . . ?
O4 Mn O4 Ba 0.0 97_666 . . . ?
Cs Mn O4 Ba 0.0 . . . . ?
Cs Mn O4 Ba 0.0 97_666 . . . ?
Ca Mn O4 Ba 0.0 2_566 . . . ?
Ca Mn O4 Ba 0.0 27_554 . . . ?
Ca Mn O4 Ba 0.0 51_564 . . . ?
Ca Mn O4 Ba 0.0 4 . . . ?
Ca Mn O4 Ba 0.0 52 . . . ?
Ba Mn O4 Ba 0.0 2_566 . . . ?
Ba Mn O4 Ba 0.0 26 . . . ?
Ba Mn O4 Ba 0.0 27_554 . . . ?
O4 Mn O4 Sr 0.0 97_666 . . . ?
Cs Mn O4 Sr 0.0 . . . . ?
Cs Mn O4 Sr 0.0 97_666 . . . ?
Ca Mn O4 Sr 0.0 2_566 . . . ?
Ca Mn O4 Sr 0.0 27_554 . . . ?
Ca Mn O4 Sr 0.0 51_564 . . . ?
Ca Mn O4 Sr 0.0 4 . . . ?
Ca Mn O4 Sr 0.0 52 . . . ?
Ba Mn O4 Sr 0.0 2_566 . . . ?
Ba Mn O4 Sr 0.0 26 . . . ?
Ba Mn O4 Sr 0.0 27_554 . . . ?
O4 Mn O4 Ce 0.0 97_666 . . . ?
Cs Mn O4 Ce 0.0 . . . . ?
Cs Mn O4 Ce 0.0 97_666 . . . ?
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```
Ca Mn O4 Ce 0.0 2_566 . . . ?
Ca Mn O4 Ce 0.0 27_554 . . . ?
Ca Mn O4 Ce 0.0 51_564 . . . ?
Ca Mn O4 Ce 0.0 4 . . . ?
Ca Mn O4 Ce 0.0 52 . . . ?
Ba Mn O4 Ce 0.0 2_566 . . . ?
Ba Mn O4 Ce 0.0 26 . . . ?
Ba Mn O4 Ce 0.0 27_554 . . . ?
O4 Mn O4 U 0.0 97_666 . . . ?
Cs Mn O4 U 0.0 . . . . ?
Cs Mn O4 U 0.0 97_666 . . . ?
Ca Mn O4 U 0.0 2_566 . . . ?
Ca Mn O4 U 0.0 27_554 . . . ?
Ca Mn O4 U 0.0 51_564 . . . ?
Ca Mn O4 U 0.0 4 . . . ?
Ca Mn O4 U 0.0 52 . . . ?
Ba Mn O4 U 0.0 2_566 . . . ?
Ba Mn O4 U 0.0 26 . . . ?
Ba Mn O4 U 0.0 27_554 . . . ?
O4 Mn O4 Bi 0.0 97_666 . . . ?
Cs Mn O4 Bi 0.0 . . . . ?
Cs Mn O4 Bi 0.0 97_666 . . . ?
Ca Mn O4 Bi 0.0 2_566 . . . ?
Ca Mn O4 Bi 0.0 27_554 . . . ?
Ca Mn O4 Bi 0.0 51_564 . . . ?
Ca Mn O4 Bi 0.0 4 . . . ?
Ca Mn O4 Bi 0.0 52 . . . ?
Ba Mn O4 Bi 0.0 2_566 . . . ?
Ba Mn O4 Bi 0.0 26 . . . ?
Ba Mn O4 Bi 0.0 27_554 . . . ?
O4 Mn O4 Nd 0.0 97_666 . . . ?
Cs Mn O4 Nd 0.0 . . . . ?
Cs Mn O4 Nd 0.0 97_666 . . . ?
Ca Mn O4 Nd 0.0 2_566 . . . ?
Ca Mn O4 Nd 0.0 27_554 . . . ?
Ca Mn O4 Nd 0.0 51_564 . . . ?
Ca Mn O4 Nd 0.0 4 . . . ?
Ca Mn O4 Nd 0.0 52 . . . ?
Ba Mn O4 Nd 0.0 2_566 . . . ?
Ba Mn O4 Nd 0.0 26 . . . ?
Ba Mn O4 Nd 0.0 27_554 . . . ?
O4 Mn O4 La 0.0 97_666 . . . ?
Cs Mn O4 La 0.0 . . . . ?
Cs Mn O4 La 0.0 97_666 . . . ?
Ca Mn O4 La 0.0 2_566 . . . ?
Ca Mn O4 La 0.0 27_554 . . . ?
Ca Mn O4 La 0.0 51_564 . . . ?
Ca Mn O4 La 0.0 4 . . . ?
Ca Mn O4 La 0.0 52 . . . ?
Ba Mn O4 La 0.0 2_566 . . . ?
Ba Mn O4 La 0.0 26 . . . ?
Ba Mn O4 La 0.0 27_554 . . . ?
O4 Mn O4 Pb -120(100) 97_666 . . 4 ?
Cs Mn O4 Pb 0.0 . . . 4 ?
Cs Mn O4 Pb -120(100) 97_666 . . 4 ?
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```
Ca Mn O4 Pb 60.0 2_566 . . 4 ?
Ca Mn O4 Pb 120.0 27_554 . . 4 ?
Ca Mn O4 Pb -60.0 51_564 . . 4 ?
Ca Mn O4 Pb 0.0 4 . . 4 ?
Ca Mn O4 Pb 180.0 52 . . 4 ?
Ba Mn O4 Pb 60.0 2_566 . . 4 ?
Ba Mn O4 Pb -120.0 26 . . 4 ?
Ba Mn O4 Pb 120.0 27_554 . . 4 ?
O4 Mn O4 Ca 0(100) 97_666 . . 26 ?
Cs Mn O4 Ca 0.0 . . . 26 ?
Cs Mn O4 Ca 0(100) 97_666 . . 26 ?
Ca Mn O4 Ca 180.0 2_566 . . 26 ?
Ca Mn O4 Ca -120.0 27_554 . . 26 ?
Ca Mn O4 Ca 60.0 51_564 . . 26 ?
Ca Mn O4 Ca 120.0 4 . . 26 ?
Ca Mn O4 Ca -60.0 52 . . 26 ?
Ba Mn O4 Ca 180.0 2_566 . . 26 ?
Ba Mn O4 Ca 0.0 26 . . 26 ?
Ba Mn O4 Ca -120.0 27_554 . . 26 ?
O4 Ba O4 Pb 0.0 97_666 . . . ?
Cs Ba O4 Pb 0.0 . . . . ?
Cs Ba O4 Pb 0.0 97_666 . . . ?
O3 Ba O4 Pb 0.0 148_565 . . . ?
O3 Ba O4 Pb 0.0 52 . . . ?
O3 Ba O4 Pb 0.0 147_556 . . . ?
O3 Ba O4 Pb 0.0 51_564 . . . ?
O3 Ba O4 Pb 0.0 98_655 . . . ?
O3 Ba O4 Pb 0.0 2_566 . . . ?
O2 Ba O4 Pb 0.0 177_556 . . . ?
O2 Ba O4 Pb 0.0 81 . . . ?
O4 Ba O4 Ca 0.0 97_666 . . . ?
Cs Ba O4 Ca 0.0 . . . . ?
Cs Ba O4 Ca 0.0 97_666 . . . ?
O3 Ba O4 Ca 0.0 148_565 . . . ?
O3 Ba O4 Ca 0.0 52 . . . ?
O3 Ba O4 Ca 0.0 147_556 . . . ?
O3 Ba O4 Ca 0.0 51_564 . . . ?
O3 Ba O4 Ca 0.0 98_655 . . . ?
O3 Ba O4 Ca 0.0 2_566 . . . ?
O2 Ba O4 Ca 0.0 177_556 . . . ?
O2 Ba O4 Ca 0.0 81 . . . ?
O4 Ba O4 Mn 0.0 97_666 . . . ?
Cs Ba O4 Mn 0.0 . . . . ?
Cs Ba O4 Mn 0.0 97_666 . . . ?
O3 Ba O4 Mn 0.0 148_565 . . . ?
O3 Ba O4 Mn 0.0 52 . . . ?
O3 Ba O4 Mn 0.0 147_556 . . . ?
O3 Ba O4 Mn 0.0 51_564 . . . ?
O3 Ba O4 Mn 0.0 98_655 . . . ?
O3 Ba O4 Mn 0.0 2_566 . . . ?
O2 Ba O4 Mn 0.0 177_556 . . . ?
O2 Ba O4 Mn 0.0 81 . . . ?
O4 Ba O4 Sr 0.0 97_666 . . . ?
Cs Ba O4 Sr 0.0 . . . . ?
Cs Ba O4 Sr 0.0 97_666 . . . ?
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```
O3 Ba O4 Sr 0.0 148_565 . . . ?
O3 Ba O4 Sr 0.0 52 . . . ?
O3 Ba O4 Sr 0.0 147_556 . . . ?
O3 Ba O4 Sr 0.0 51_564 . . . ?
O3 Ba O4 Sr 0.0 98_655 . . . ?
O3 Ba O4 Sr 0.0 2_566 . . . ?
O2 Ba O4 Sr 0.0 177_556 . . . ?
O2 Ba O4 Sr 0.0 81 . . . ?
O4 Ba O4 Ce 0.0 97_666 . . . ?
Cs Ba O4 Ce 0.0 . . . . ?
Cs Ba O4 Ce 0.0 97_666 . . . ?
O3 Ba O4 Ce 0.0 148_565 . . . ?
O3 Ba O4 Ce 0.0 52 . . . ?
O3 Ba O4 Ce 0.0 147_556 . . . ?
O3 Ba O4 Ce 0.0 51_564 . . . ?
O3 Ba O4 Ce 0.0 98_655 . . . ?
O3 Ba O4 Ce 0.0 2_566 . . . ?
O2 Ba O4 Ce 0.0 177_556 . . . ?
O2 Ba O4 Ce 0.0 81 . . . ?
O4 Ba O4 U 0.0 97_666 . . . ?
Cs Ba O4 U 0.0 . . . . ?
Cs Ba O4 U 0.0 97_666 . . . ?
O3 Ba O4 U 0.0 148_565 . . . ?
O3 Ba O4 U 0.0 52 . . . ?
O3 Ba O4 U 0.0 147_556 . . . ?
O3 Ba O4 U 0.0 51_564 . . . ?
O3 Ba O4 U 0.0 98_655 . . . ?
O3 Ba O4 U 0.0 2_566 . . . ?
O2 Ba O4 U 0.0 177_556 . . . ?
O2 Ba O4 U 0.0 81 . . . ?
O4 Ba O4 Bi 0.0 97_666 . . . ?
Cs Ba O4 Bi 0.0 . . . . ?
Cs Ba O4 Bi 0.0 97_666 . . . ?
O3 Ba O4 Bi 0.0 148_565 . . . ?
O3 Ba O4 Bi 0.0 52 . . . ?
O3 Ba O4 Bi 0.0 147_556 . . . ?
O3 Ba O4 Bi 0.0 51_564 . . . ?
O3 Ba O4 Bi 0.0 98_655 . . . ?
O3 Ba O4 Bi 0.0 2_566 . . . ?
O2 Ba O4 Bi 0.0 177_556 . . . ?
O2 Ba O4 Bi 0.0 81 . . . ?
O4 Ba O4 Nd 0.0 97_666 . . . ?
Cs Ba O4 Nd 0.0 . . . . ?
Cs Ba O4 Nd 0.0 97_666 . . . ?
O3 Ba O4 Nd 0.0 148_565 . . . ?
O3 Ba O4 Nd 0.0 52 . . . ?
O3 Ba O4 Nd 0.0 147_556 . . . ?
O3 Ba O4 Nd 0.0 51_564 . . . ?
O3 Ba O4 Nd 0.0 98_655 . . . ?
O3 Ba O4 Nd 0.0 2_566 . . . ?
O2 Ba O4 Nd 0.0 177_556 . . . ?
O2 Ba O4 Nd 0.0 81 . . . ?
O4 Ba O4 La 0.0 97_666 . . . ?
Cs Ba O4 La 0.0 . . . . ?
Cs Ba O4 La 0.0 97_666 . . . ?
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O3 Ba O4 La 0.0 148_565 . . . ?
O3 Ba O4 La 0.0 52 . . . ?
O3 Ba O4 La 0.0 147_556 . . . ?
O3 Ba O4 La 0.0 51_564 . . . ?
O3 Ba O4 La 0.0 98_655 . . . ?
O3 Ba O4 La 0.0 2_566 . . . ?
O2 Ba O4 La 0.0 177_556 . . . ?
O2 Ba O4 La 0.0 81 . . . ?
O4 Ba O4 Pb -120(100) 97_666 . . 4 ?
Cs Ba O4 Pb 0.0 . . . 4 ?
Cs Ba O4 Pb -120(100) 97_666 . . 4 ?
O3 Ba O4 Pb 180.0 148_565 . . 4 ?
O3 Ba O4 Pb 0.0 52 . . 4 ?
O3 Ba O4 Pb -60.0 147_556 . . 4 ?
O3 Ba O4 Pb 120.0 51_564 . . 4 ?
O3 Ba O4 Pb 60.0 98_655 . . 4 ?
O3 Ba O4 Pb -120.0 2_566 . . 4 ?
O2 Ba O4 Pb 120.0 177_556 . . 4 ?
O2 Ba O4 Pb -60.0 81 . . 4 ?
O4 Ba O4 Ca 0(100) 97_666 . . 26 ?
Cs Ba O4 Ca 0.0 . . . 26 ?
Cs Ba O4 Ca 0(100) 97_666 . . 26 ?
O3 Ba O4 Ca -60.0 148_565 . . 26 ?
O3 Ba O4 Ca 120.0 52 . . 26 ?
O3 Ba O4 Ca 60.0 147_556 . . 26 ?
O3 Ba O4 Ca -120.0 51_564 . . 26 ?
O3 Ba O4 Ca 180.0 98_655 . . 26 ?
O3 Ba O4 Ca 0.0 2_566 . . 26 ?
O2 Ba O4 Ca -120.0 177_556 . . 26 ?
O2 Ba O4 Ca 60.0 81 . . 26 ?
O4 Sr O4 Pb 0.0 97_666 . . . ?
Cs Sr O4 Pb 0.0 . . . . ?
Cs Sr O4 Pb 0.0 97_666 . . . ?
O3 Sr O4 Pb 0.0 148_565 . . . ?
O3 Sr O4 Pb 0.0 52 . . . ?
O3 Sr O4 Pb 0.0 147_556 . . . ?
O3 Sr O4 Pb 0.0 51_564 . . . ?
O3 Sr O4 Pb 0.0 98_655 . . . ?
O3 Sr O4 Pb 0.0 2_566 . . . ?
O2 Sr O4 Pb 0.0 177_556 . . . ?
O2 Sr O4 Pb 0.0 81 . . . ?
O4 Sr O4 Ca 0.0 97_666 . . . ?
Cs Sr O4 Ca 0.0 . . . . ?
Cs Sr O4 Ca 0.0 97_666 . . . ?
O3 Sr O4 Ca 0.0 148_565 . . . ?
O3 Sr O4 Ca 0.0 52 . . . ?
O3 Sr O4 Ca 0.0 147_556 . . . ?
O3 Sr O4 Ca 0.0 51_564 . . . ?
O3 Sr O4 Ca 0.0 98_655 . . . ?
O3 Sr O4 Ca 0.0 2_566 . . . ?
O2 Sr O4 Ca 0.0 177_556 . . . ?
O2 Sr O4 Ca 0.0 81 . . . ?
O4 Sr O4 Mn 0.0 97_666 . . . ?
Cs Sr O4 Mn 0.0 . . . . ?
Cs Sr O4 Mn 0.0 97_666 . . . ?
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O3 Sr O4 Mn 0.0 148_565 . . . ?
O3 Sr O4 Mn 0.0 52 . . . ?
O3 Sr O4 Mn 0.0 147_556 . . . ?
O3 Sr O4 Mn 0.0 51_564 . . . ?
O3 Sr O4 Mn 0.0 98_655 . . . ?
O3 Sr O4 Mn 0.0 2_566 . . . ?
O2 Sr O4 Mn 0.0 177_556 . . . ?
O2 Sr O4 Mn 0.0 81 . . . ?
O4 Sr O4 Ba 0.0 97_666 . . . ?
Cs Sr O4 Ba 0.0 . . . . ?
Cs Sr O4 Ba 0.0 97_666 . . . ?
O3 Sr O4 Ba 0.0 148_565 . . . ?
O3 Sr O4 Ba 0.0 52 . . . ?
O3 Sr O4 Ba 0.0 147_556 . . . ?
O3 Sr O4 Ba 0.0 51_564 . . . ?
O3 Sr O4 Ba 0.0 98_655 . . . ?
O3 Sr O4 Ba 0.0 2_566 . . . ?
O2 Sr O4 Ba 0.0 177_556 . . . ?
O2 Sr O4 Ba 0.0 81 . . . ?
O4 Sr O4 Ce 0.0 97_666 . . . ?
Cs Sr O4 Ce 0.0 . . . . ?
Cs Sr O4 Ce 0.0 97_666 . . . ?
O3 Sr O4 Ce 0.0 148_565 . . . ?
O3 Sr O4 Ce 0.0 52 . . . ?
O3 Sr O4 Ce 0.0 147_556 . . . ?
O3 Sr O4 Ce 0.0 51_564 . . . ?
O3 Sr O4 Ce 0.0 98_655 . . . ?
O3 Sr O4 Ce 0.0 2_566 . . . ?
O2 Sr O4 Ce 0.0 177_556 . . . ?
O2 Sr O4 Ce 0.0 81 . . . ?
O4 Sr O4 U 0.0 97_666 . . . ?
Cs Sr O4 U 0.0 . . . . ?
Cs Sr O4 U 0.0 97_666 . . . ?
O3 Sr O4 U 0.0 148_565 . . . ?
O3 Sr O4 U 0.0 52 . . . ?
O3 Sr O4 U 0.0 147_556 . . . ?
O3 Sr O4 U 0.0 51_564 . . . ?
O3 Sr O4 U 0.0 98_655 . . . ?
O3 Sr O4 U 0.0 2_566 . . . ?
O2 Sr O4 U 0.0 177_556 . . . ?
O2 Sr O4 U 0.0 81 . . . ?
O4 Sr O4 Bi 0.0 97_666 . . . ?
Cs Sr O4 Bi 0.0 . . . . ?
Cs Sr O4 Bi 0.0 97_666 . . . ?
O3 Sr O4 Bi 0.0 148_565 . . . ?
O3 Sr O4 Bi 0.0 52 . . . ?
O3 Sr O4 Bi 0.0 147_556 . . . ?
O3 Sr O4 Bi 0.0 51_564 . . . ?
O3 Sr O4 Bi 0.0 98_655 . . . ?
O3 Sr O4 Bi 0.0 2_566 . . . ?
O2 Sr O4 Bi 0.0 177_556 . . . ?
O2 Sr O4 Bi 0.0 81 . . . ?
O4 Sr O4 Nd 0.0 97_666 . . . ?
Cs Sr O4 Nd 0.0 . . . . ?
Cs Sr O4 Nd 0.0 97_666 . . . ?
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```
O3 Sr O4 Nd 0.0 148_565 . . . ?
O3 Sr O4 Nd 0.0 52 . . . ?
O3 Sr O4 Nd 0.0 147_556 . . . ?
O3 Sr O4 Nd 0.0 51_564 . . . ?
O3 Sr O4 Nd 0.0 98_655 . . . ?
O3 Sr O4 Nd 0.0 2_566 . . . ?
O2 Sr O4 Nd 0.0 177_556 . . . ?
O2 Sr O4 Nd 0.0 81 . . . ?
O4 Sr O4 La 0.0 97_666 . . . ?
Cs Sr O4 La 0.0 . . . . ?
Cs Sr O4 La 0.0 97_666 . . . ?
O3 Sr O4 La 0.0 148_565 . . . ?
O3 Sr O4 La 0.0 52 . . . ?
O3 Sr O4 La 0.0 147_556 . . . ?
O3 Sr O4 La 0.0 51_564 . . . ?
O3 Sr O4 La 0.0 98_655 . . . ?
O3 Sr O4 La 0.0 2_566 . . . ?
O2 Sr O4 La 0.0 177_556 . . . ?
O2 Sr O4 La 0.0 81 . . . ?
O4 Sr O4 Pb -120(100) 97_666 . . 4 ?
Cs Sr O4 Pb 0.0 . . . 4 ?
Cs Sr O4 Pb -120(100) 97_666 . . 4 ?
O3 Sr O4 Pb 180.0 148_565 . . 4 ?
O3 Sr O4 Pb 0.0 52 . . 4 ?
O3 Sr O4 Pb -60.0 147_556 . . 4 ?
O3 Sr O4 Pb 120.0 51_564 . . 4 ?
O3 Sr O4 Pb 60.0 98_655 . . 4 ?
O3 Sr O4 Pb -120.0 2_566 . . 4 ?
O2 Sr O4 Pb 120.0 177_556 . . 4 ?
O2 Sr O4 Pb -60.0 81 . . 4 ?
O4 Sr O4 Ca 0(100) 97_666 . . 26 ?
Cs Sr O4 Ca 0.0 . . . 26 ?
Cs Sr O4 Ca 0(100) 97_666 . . 26 ?
O3 Sr O4 Ca -60.0 148_565 . . 26 ?
O3 Sr O4 Ca 120.0 52 . . 26 ?
O3 Sr O4 Ca 60.0 147_556 . . 26 ?
O3 Sr O4 Ca -120.0 51_564 . . 26 ?
O3 Sr O4 Ca 180.0 98_655 . . 26 ?
O3 Sr O4 Ca 0.0 2_566 . . 26 ?
O2 Sr O4 Ca -120.0 177_556 . . 26 ?
O2 Sr O4 Ca 60.0 81 . . 26 ?
O4 Ce O4 Pb 0.0 97_666 . . . ?
Cs Ce O4 Pb 0.0 . . . . ?
Cs Ce O4 Pb 0.0 97_666 . . . ?
O3 Ce O4 Pb 0.0 148_565 . . . ?
O3 Ce O4 Pb 0.0 52 . . . ?
O3 Ce O4 Pb 0.0 147_556 . . . ?
O3 Ce O4 Pb 0.0 51_564 . . . ?
O3 Ce O4 Pb 0.0 98_655 . . . ?
O3 Ce O4 Pb 0.0 2_566 . . . ?
O2 Ce O4 Pb 0.0 177_556 . . . ?
O2 Ce O4 Pb 0.0 81 . . . ?
O4 Ce O4 Ca 0.0 97_666 . . . ?
Cs Ce O4 Ca 0.0 . . . . ?
Cs Ce O4 Ca 0.0 97_666 . . . ?
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```
O3 Ce O4 Ca 0.0 148_565 . . . ?
O3 Ce O4 Ca 0.0 52 . . . ?
O3 Ce O4 Ca 0.0 147_556 . . . ?
O3 Ce O4 Ca 0.0 51_564 . . . ?
O3 Ce O4 Ca 0.0 98_655 . . . ?
O3 Ce O4 Ca 0.0 2_566 . . . ?
O2 Ce O4 Ca 0.0 177_556 . . . ?
O2 Ce O4 Ca 0.0 81 . . . ?
O4 Ce O4 Mn 0.0 97_666 . . . ?
Cs Ce O4 Mn 0.0 . . . . ?
Cs Ce O4 Mn 0.0 97_666 . . . ?
O3 Ce O4 Mn 0.0 148_565 . . . ?
O3 Ce O4 Mn 0.0 52 . . . ?
O3 Ce O4 Mn 0.0 147_556 . . . ?
O3 Ce O4 Mn 0.0 51_564 . . . ?
O3 Ce O4 Mn 0.0 98_655 . . . ?
O3 Ce O4 Mn 0.0 2_566 . . . ?
O2 Ce O4 Mn 0.0 177_556 . . . ?
O2 Ce O4 Mn 0.0 81 . . . ?
O4 Ce O4 Ba 0.0 97_666 . . . ?
Cs Ce O4 Ba 0.0 . . . . ?
Cs Ce O4 Ba 0.0 97_666 . . . ?
O3 Ce O4 Ba 0.0 148_565 . . . ?
O3 Ce O4 Ba 0.0 52 . . . ?
O3 Ce O4 Ba 0.0 147_556 . . . ?
O3 Ce O4 Ba 0.0 51_564 . . . ?
O3 Ce O4 Ba 0.0 98_655 . . . ?
O3 Ce O4 Ba 0.0 2_566 . . . ?
O2 Ce O4 Ba 0.0 177_556 . . . ?
O2 Ce O4 Ba 0.0 81 . . . ?
O4 Ce O4 Sr 0.0 97_666 . . . ?
Cs Ce O4 Sr 0.0 . . . . ?
Cs Ce O4 Sr 0.0 97_666 . . . ?
O3 Ce O4 Sr 0.0 148_565 . . . ?
O3 Ce O4 Sr 0.0 52 . . . ?
O3 Ce O4 Sr 0.0 147_556 . . . ?
O3 Ce O4 Sr 0.0 51_564 . . . ?
O3 Ce O4 Sr 0.0 98_655 . . . ?
O3 Ce O4 Sr 0.0 2_566 . . . ?
O2 Ce O4 Sr 0.0 177_556 . . . ?
O2 Ce O4 Sr 0.0 81 . . . ?
O4 Ce O4 U 0.0 97_666 . . . ?
Cs Ce O4 U 0.0 . . . . ?
Cs Ce O4 U 0.0 97_666 . . . ?
O3 Ce O4 U 0.0 148_565 . . . ?
O3 Ce O4 U 0.0 52 . . . ?
O3 Ce O4 U 0.0 147_556 . . . ?
O3 Ce O4 U 0.0 51_564 . . . ?
O3 Ce O4 U 0.0 98_655 . . . ?
O3 Ce O4 U 0.0 2_566 . . . ?
O2 Ce O4 U 0.0 177_556 . . . ?
O2 Ce O4 U 0.0 81 . . . ?
O4 Ce O4 Bi 0.0 97_666 . . . ?
Cs Ce O4 Bi 0.0 . . . . ?
Cs Ce O4 Bi 0.0 97_666 . . . ?
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```
O3 Ce O4 Bi 0.0 148_565 . . . ?
O3 Ce O4 Bi 0.0 52 . . . ?
O3 Ce O4 Bi 0.0 147_556 . . . ?
O3 Ce O4 Bi 0.0 51_564 . . . ?
O3 Ce O4 Bi 0.0 98_655 . . . ?
O3 Ce O4 Bi 0.0 2_566 . . . ?
O2 Ce O4 Bi 0.0 177_556 . . . ?
O2 Ce O4 Bi 0.0 81 . . . ?
O4 Ce O4 Nd 0.0 97_666 . . . ?
Cs Ce O4 Nd 0.0 . . . . ?
Cs Ce O4 Nd 0.0 97_666 . . . ?
O3 Ce O4 Nd 0.0 148_565 . . . ?
O3 Ce O4 Nd 0.0 52 . . . ?
O3 Ce O4 Nd 0.0 147_556 . . . ?
O3 Ce O4 Nd 0.0 51_564 . . . ?
O3 Ce O4 Nd 0.0 98_655 . . . ?
O3 Ce O4 Nd 0.0 2_566 . . . ?
O2 Ce O4 Nd 0.0 177_556 . . . ?
O2 Ce O4 Nd 0.0 81 . . . ?
O4 Ce O4 La 0.0 97_666 . . . ?
Cs Ce O4 La 0.0 . . . . ?
Cs Ce O4 La 0.0 97_666 . . . ?
O3 Ce O4 La 0.0 148_565 . . . ?
O3 Ce O4 La 0.0 52 . . . ?
O3 Ce O4 La 0.0 147_556 . . . ?
O3 Ce O4 La 0.0 51_564 . . . ?
O3 Ce O4 La 0.0 98_655 . . . ?
O3 Ce O4 La 0.0 2_566 . . . ?
O2 Ce O4 La 0.0 177_556 . . . ?
O2 Ce O4 La 0.0 81 . . . ?
O4 Ce O4 Pb -120(100) 97_666 . . 4 ?
Cs Ce O4 Pb 0.0 . . . 4 ?
Cs Ce O4 Pb -120(100) 97_666 . . 4 ?
O3 Ce O4 Pb 180.0 148_565 . . 4 ?
O3 Ce O4 Pb 0.0 52 . . 4 ?
O3 Ce O4 Pb -60.0 147_556 . . 4 ?
O3 Ce O4 Pb 120.0 51_564 . . 4 ?
O3 Ce O4 Pb 60.0 98_655 . . 4 ?
O3 Ce O4 Pb -120.0 2_566 . . 4 ?
O2 Ce O4 Pb 120.0 177_556 . . 4 ?
O2 Ce O4 Pb -60.0 81 . . 4 ?
O4 Ce O4 Ca 0(100) 97_666 . . 26 ?
Cs Ce O4 Ca 0.0 . . . 26 ?
Cs Ce O4 Ca 0(100) 97_666 . . 26 ?
O3 Ce O4 Ca -60.0 148_565 . . 26 ?
O3 Ce O4 Ca 120.0 52 . . 26 ?
O3 Ce O4 Ca 60.0 147_556 . . 26 ?
O3 Ce O4 Ca -120.0 51_564 . . 26 ?
O3 Ce O4 Ca 180.0 98_655 . . 26 ?
O3 Ce O4 Ca 0.0 2_566 . . 26 ?
O2 Ce O4 Ca -120.0 177_556 . . 26 ?
O2 Ce O4 Ca 60.0 81 . . 26 ?
O4 U O4 Pb 0.0 97_666 . . . ?
Cs U O4 Pb 0.0 . . . . ?
Cs U O4 Pb 0.0 97_666 . . . ?
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```
O3 U O4 Pb 0.0 148_565 . . . ?
O3 U O4 Pb 0.0 52 . . . ?
O3 U O4 Pb 0.0 147_556 . . . ?
O3 U O4 Pb 0.0 51_564 . . . ?
O3 U O4 Pb 0.0 98_655 . . . ?
O3 U O4 Pb 0.0 2_566 . . . ?
O2 U O4 Pb 0.0 177_556 . . . ?
O2 U O4 Pb 0.0 81 . . . ?
O4 U O4 Ca 0.0 97_666 . . . ?
Cs U O4 Ca 0.0 . . . . ?
Cs U O4 Ca 0.0 97_666 . . . ?
O3 U O4 Ca 0.0 148_565 . . . ?
O3 U O4 Ca 0.0 52 . . . ?
O3 U O4 Ca 0.0 147_556 . . . ?
O3 U O4 Ca 0.0 51_564 . . . ?
O3 U O4 Ca 0.0 98_655 . . . ?
O3 U O4 Ca 0.0 2_566 . . . ?
O2 U O4 Ca 0.0 177_556 . . . ?
O2 U O4 Ca 0.0 81 . . . ?
O4 U O4 Mn 0.0 97_666 . . . ?
Cs U O4 Mn 0.0 . . . . ?
Cs U O4 Mn 0.0 97_666 . . . ?
O3 U O4 Mn 0.0 148_565 . . . ?
O3 U O4 Mn 0.0 52 . . . ?
O3 U O4 Mn 0.0 147_556 . . . ?
O3 U O4 Mn 0.0 51_564 . . . ?
O3 U O4 Mn 0.0 98_655 . . . ?
O3 U O4 Mn 0.0 2_566 . . . ?
O2 U O4 Mn 0.0 177_556 . . . ?
O2 U O4 Mn 0.0 81 . . . ?
O4 U O4 Ba 0.0 97_666 . . . ?
Cs U O4 Ba 0.0 . . . . ?
Cs U O4 Ba 0.0 97_666 . . . ?
O3 U O4 Ba 0.0 148_565 . . . ?
O3 U O4 Ba 0.0 52 . . . ?
O3 U O4 Ba 0.0 147_556 . . . ?
O3 U O4 Ba 0.0 51_564 . . . ?
O3 U O4 Ba 0.0 98_655 . . . ?
O3 U O4 Ba 0.0 2_566 . . . ?
O2 U O4 Ba 0.0 177_556 . . . ?
O2 U O4 Ba 0.0 81 . . . ?
O4 U O4 Sr 0.0 97_666 . . . ?
Cs U O4 Sr 0.0 . . . . ?
Cs U O4 Sr 0.0 97_666 . . . ?
O3 U O4 Sr 0.0 148_565 . . . ?
O3 U O4 Sr 0.0 52 . . . ?
O3 U O4 Sr 0.0 147_556 . . . ?
O3 U O4 Sr 0.0 51_564 . . . ?
O3 U O4 Sr 0.0 98_655 . . . ?
O3 U O4 Sr 0.0 2_566 . . . ?
O2 U O4 Sr 0.0 177_556 . . . ?
O2 U O4 Sr 0.0 81 . . . ?
O4 U O4 Ce 0.0 97_666 . . . ?
Cs U O4 Ce 0.0 . . . . ?
Cs U O4 Ce 0.0 97_666 . . . ?
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```
O3 U O4 Ce 0.0 148_565 . . . ?
O3 U O4 Ce 0.0 52 . . . ?
O3 U O4 Ce 0.0 147_556 . . . ?
O3 U O4 Ce 0.0 51_564 . . . ?
O3 U O4 Ce 0.0 98_655 . . . ?
O3 U O4 Ce 0.0 2_566 . . . ?
O2 U O4 Ce 0.0 177_556 . . . ?
O2 U O4 Ce 0.0 81 . . . ?
O4 U O4 Bi 0.0 97_666 . . . ?
Cs U O4 Bi 0.0 . . . . ?
Cs U O4 Bi 0.0 97_666 . . . ?
O3 U O4 Bi 0.0 148_565 . . . ?
O3 U O4 Bi 0.0 52 . . . ?
O3 U O4 Bi 0.0 147_556 . . . ?
O3 U O4 Bi 0.0 51_564 . . . ?
O3 U O4 Bi 0.0 98_655 . . . ?
O3 U O4 Bi 0.0 2_566 . . . ?
O2 U O4 Bi 0.0 177_556 . . . ?
O2 U O4 Bi 0.0 81 . . . ?
O4 U O4 Nd 0.0 97_666 . . . ?
Cs U O4 Nd 0.0 . . . . ?
Cs U O4 Nd 0.0 97_666 . . . ?
O3 U O4 Nd 0.0 148_565 . . . ?
O3 U O4 Nd 0.0 52 . . . ?
O3 U O4 Nd 0.0 147_556 . . . ?
O3 U O4 Nd 0.0 51_564 . . . ?
O3 U O4 Nd 0.0 98_655 . . . ?
O3 U O4 Nd 0.0 2_566 . . . ?
O2 U O4 Nd 0.0 177_556 . . . ?
O2 U O4 Nd 0.0 81 . . . ?
O4 U O4 La 0.0 97_666 . . . ?
Cs U O4 La 0.0 . . . . ?
Cs U O4 La 0.0 97_666 . . . ?
O3 U O4 La 0.0 148_565 . . . ?
O3 U O4 La 0.0 52 . . . ?
O3 U O4 La 0.0 147_556 . . . ?
O3 U O4 La 0.0 51_564 . . . ?
O3 U O4 La 0.0 98_655 . . . ?
O3 U O4 La 0.0 2_566 . . . ?
O2 U O4 La 0.0 177_556 . . . ?
O2 U O4 La 0.0 81 . . . ?
O4 U O4 Pb -120(100) 97_666 . . 4 ?
Cs U O4 Pb 0.0 . . . 4 ?
Cs U O4 Pb -120(100) 97_666 . . 4 ?
O3 U O4 Pb 180.0 148_565 . . 4 ?
O3 U O4 Pb 0.0 52 . . 4 ?
O3 U O4 Pb -60.0 147_556 . . 4 ?
O3 U O4 Pb 120.0 51_564 . . 4 ?
O3 U O4 Pb 60.0 98_655 . . 4 ?
O3 U O4 Pb -120.0 2_566 . . 4 ?
O2 U O4 Pb 120.0 177_556 . . 4 ?
O2 U O4 Pb -60.0 81 . . 4 ?
O4 U O4 Ca 0(100) 97_666 . . 26 ?
Cs U O4 Ca 0.0 . . . 26 ?
Cs U O4 Ca 0(100) 97_666 . . 26 ?
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O3 U O4 Ca -60.0 148_565 . . 26 ?
O3 U O4 Ca 120.0 52 . . 26 ?
O3 U O4 Ca 60.0 147_556 . . 26 ?
O3 U O4 Ca -120.0 51_564 . . 26 ?
O3 U O4 Ca 180.0 98_655 . . 26 ?
O3 U O4 Ca 0.0 2_566 . . 26 ?
O2 U O4 Ca -120.0 177_556 . . 26 ?
O2 U O4 Ca 60.0 81 . . 26 ?
O4 Bi O4 Pb 0.0 97_666 . . . ?
Cs Bi O4 Pb 0.0 . . . . ?
Cs Bi O4 Pb 0.0 97_666 . . . ?
O3 Bi O4 Pb 0.0 148_565 . . . ?
O3 Bi O4 Pb 0.0 52 . . . ?
O3 Bi O4 Pb 0.0 147_556 . . . ?
O3 Bi O4 Pb 0.0 51_564 . . . ?
O3 Bi O4 Pb 0.0 98_655 . . . ?
O3 Bi O4 Pb 0.0 2_566 . . . ?
O2 Bi O4 Pb 0.0 177_556 . . . ?
O2 Bi O4 Pb 0.0 81 . . . ?
O4 Bi O4 Ca 0.0 97_666 . . . ?
Cs Bi O4 Ca 0.0 . . . . ?
Cs Bi O4 Ca 0.0 97_666 . . . ?
O3 Bi O4 Ca 0.0 148_565 . . . ?
O3 Bi O4 Ca 0.0 52 . . . ?
O3 Bi O4 Ca 0.0 147_556 . . . ?
O3 Bi O4 Ca 0.0 51_564 . . . ?
O3 Bi O4 Ca 0.0 98_655 . . . ?
O3 Bi O4 Ca 0.0 2_566 . . . ?
O2 Bi O4 Ca 0.0 177_556 . . . ?
O2 Bi O4 Ca 0.0 81 . . . ?
O4 Bi O4 Mn 0.0 97_666 . . . ?
Cs Bi O4 Mn 0.0 . . . . ?
Cs Bi O4 Mn 0.0 97_666 . . . ?
O3 Bi O4 Mn 0.0 148_565 . . . ?
O3 Bi O4 Mn 0.0 52 . . . ?
O3 Bi O4 Mn 0.0 147_556 . . . ?
O3 Bi O4 Mn 0.0 51_564 . . . ?
O3 Bi O4 Mn 0.0 98_655 . . . ?
O3 Bi O4 Mn 0.0 2_566 . . . ?
O2 Bi O4 Mn 0.0 177_556 . . . ?
O2 Bi O4 Mn 0.0 81 . . . ?
O4 Bi O4 Ba 0.0 97_666 . . . ?
Cs Bi O4 Ba 0.0 . . . . ?
Cs Bi O4 Ba 0.0 97_666 . . . ?
O3 Bi O4 Ba 0.0 148_565 . . . ?
O3 Bi O4 Ba 0.0 52 . . . ?
O3 Bi O4 Ba 0.0 147_556 . . . ?
O3 Bi O4 Ba 0.0 51_564 . . . ?
O3 Bi O4 Ba 0.0 98_655 . . . ?
O3 Bi O4 Ba 0.0 2_566 . . . ?
O2 Bi O4 Ba 0.0 177_556 . . . ?
O2 Bi O4 Ba 0.0 81 . . . ?
O4 Bi O4 Sr 0.0 97_666 . . . ?
Cs Bi O4 Sr 0.0 . . . . ?
Cs Bi O4 Sr 0.0 97_666 . . . ?
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O3 Bi O4 Sr 0.0 148_565 . . . ?
O3 Bi O4 Sr 0.0 52 . . . ?
O3 Bi O4 Sr 0.0 147_556 . . . ?
O3 Bi O4 Sr 0.0 51_564 . . . ?
O3 Bi O4 Sr 0.0 98_655 . . . ?
O3 Bi O4 Sr 0.0 2_566 . . . ?
O2 Bi O4 Sr 0.0 177_556 . . . ?
O2 Bi O4 Sr 0.0 81 . . . ?
O4 Bi O4 Ce 0.0 97_666 . . . ?
Cs Bi O4 Ce 0.0 . . . . ?
Cs Bi O4 Ce 0.0 97_666 . . . ?
O3 Bi O4 Ce 0.0 148_565 . . . ?
O3 Bi O4 Ce 0.0 52 . . . ?
O3 Bi O4 Ce 0.0 147_556 . . . ?
O3 Bi O4 Ce 0.0 51_564 . . . ?
O3 Bi O4 Ce 0.0 98_655 . . . ?
O3 Bi O4 Ce 0.0 2_566 . . . ?
O2 Bi O4 Ce 0.0 177_556 . . . ?
O2 Bi O4 Ce 0.0 81 . . . ?
O4 Bi O4 U 0.0 97_666 . . . ?
Cs Bi O4 U 0.0 . . . . ?
Cs Bi O4 U 0.0 97_666 . . . ?
O3 Bi O4 U 0.0 148_565 . . . ?
O3 Bi O4 U 0.0 52 . . . ?
O3 Bi O4 U 0.0 147_556 . . . ?
O3 Bi O4 U 0.0 51_564 . . . ?
O3 Bi O4 U 0.0 98_655 . . . ?
O3 Bi O4 U 0.0 2_566 . . . ?
O2 Bi O4 U 0.0 177_556 . . . ?
O2 Bi O4 U 0.0 81 . . . ?
O4 Bi O4 Nd 0.0 97_666 . . . ?
Cs Bi O4 Nd 0.0 . . . . ?
Cs Bi O4 Nd 0.0 97_666 . . . ?
O3 Bi O4 Nd 0.0 148_565 . . . ?
O3 Bi O4 Nd 0.0 52 . . . ?
O3 Bi O4 Nd 0.0 147_556 . . . ?
O3 Bi O4 Nd 0.0 51_564 . . . ?
O3 Bi O4 Nd 0.0 98_655 . . . ?
O3 Bi O4 Nd 0.0 2_566 . . . ?
O2 Bi O4 Nd 0.0 177_556 . . . ?
O2 Bi O4 Nd 0.0 81 . . . ?
O4 Bi O4 La 0.0 97_666 . . . ?
Cs Bi O4 La 0.0 . . . . ?
Cs Bi O4 La 0.0 97_666 . . . ?
O3 Bi O4 La 0.0 148_565 . . . ?
O3 Bi O4 La 0.0 52 . . . ?
O3 Bi O4 La 0.0 147_556 . . . ?
O3 Bi O4 La 0.0 51_564 . . . ?
O3 Bi O4 La 0.0 98_655 . . . ?
O3 Bi O4 La 0.0 2_566 . . . ?
O2 Bi O4 La 0.0 177_556 . . . ?
O2 Bi O4 La 0.0 81 . . . ?
O4 Bi O4 Pb -120(100) 97_666 . . 4 ?
Cs Bi O4 Pb 0.0 . . . 4 ?
Cs Bi O4 Pb -120(100) 97_666 . . 4 ?
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O3 Bi O4 Pb 180.0 148_565 . . 4 ?
O3 Bi O4 Pb 0.0 52 . . 4 ?
O3 Bi O4 Pb -60.0 147_556 . . 4 ?
O3 Bi O4 Pb 120.0 51_564 . . 4 ?
O3 Bi O4 Pb 60.0 98_655 . . 4 ?
O3 Bi O4 Pb -120.0 2_566 . . 4 ?
O2 Bi O4 Pb 120.0 177_556 . . 4 ?
O2 Bi O4 Pb -60.0 81 . . 4 ?
O4 Bi O4 Ca 0(100) 97_666 . . 26 ?
Cs Bi O4 Ca 0.0 . . . 26 ?
Cs Bi O4 Ca 0(100) 97_666 . . 26 ?
O3 Bi O4 Ca -60.0 148_565 . . 26 ?
O3 Bi O4 Ca 120.0 52 . . 26 ?
O3 Bi O4 Ca 60.0 147_556 . . 26 ?
O3 Bi O4 Ca -120.0 51_564 . . 26 ?
O3 Bi O4 Ca 180.0 98_655 . . 26 ?
O3 Bi O4 Ca 0.0 2_566 . . 26 ?
O2 Bi O4 Ca -120.0 177_556 . . 26 ?
O2 Bi O4 Ca 60.0 81 . . 26 ?
O4 Nd O4 Pb 0.0 97_666 . . . ?
Cs Nd O4 Pb 0.0 . . . . ?
Cs Nd O4 Pb 0.0 97_666 . . . ?
O3 Nd O4 Pb 0.0 148_565 . . . ?
O3 Nd O4 Pb 0.0 52 . . . ?
O3 Nd O4 Pb 0.0 147_556 . . . ?
O3 Nd O4 Pb 0.0 51_564 . . . ?
O3 Nd O4 Pb 0.0 98_655 . . . ?
O3 Nd O4 Pb 0.0 2_566 . . . ?
O2 Nd O4 Pb 0.0 177_556 . . . ?
O2 Nd O4 Pb 0.0 81 . . . ?
O4 Nd O4 Ca 0.0 97_666 . . . ?
Cs Nd O4 Ca 0.0 . . . . ?
Cs Nd O4 Ca 0.0 97_666 . . . ?
O3 Nd O4 Ca 0.0 148_565 . . . ?
O3 Nd O4 Ca 0.0 52 . . . ?
O3 Nd O4 Ca 0.0 147_556 . . . ?
O3 Nd O4 Ca 0.0 51_564 . . . ?
O3 Nd O4 Ca 0.0 98_655 . . . ?
O3 Nd O4 Ca 0.0 2_566 . . . ?
O2 Nd O4 Ca 0.0 177_556 . . . ?
O2 Nd O4 Ca 0.0 81 . . . ?
O4 Nd O4 Mn 0.0 97_666 . . . ?
Cs Nd O4 Mn 0.0 . . . . ?
Cs Nd O4 Mn 0.0 97_666 . . . ?
O3 Nd O4 Mn 0.0 148_565 . . . ?
O3 Nd O4 Mn 0.0 52 . . . ?
O3 Nd O4 Mn 0.0 147_556 . . . ?
O3 Nd O4 Mn 0.0 51_564 . . . ?
O3 Nd O4 Mn 0.0 98_655 . . . ?
O3 Nd O4 Mn 0.0 2_566 . . . ?
O2 Nd O4 Mn 0.0 177_556 . . . ?
O2 Nd O4 Mn 0.0 81 . . . ?
O4 Nd O4 Ba 0.0 97_666 . . . ?
Cs Nd O4 Ba 0.0 . . . . ?
Cs Nd O4 Ba 0.0 97_666 . . . ?
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O3 Nd O4 Ba 0.0 148_565 . . . ?
O3 Nd O4 Ba 0.0 52 . . . ?
O3 Nd O4 Ba 0.0 147_556 . . . ?
O3 Nd O4 Ba 0.0 51_564 . . . ?
O3 Nd O4 Ba 0.0 98_655 . . . ?
O3 Nd O4 Ba 0.0 2_566 . . . ?
O2 Nd O4 Ba 0.0 177_556 . . . ?
O2 Nd O4 Ba 0.0 81 . . . ?
O4 Nd O4 Sr 0.0 97_666 . . . ?
Cs Nd O4 Sr 0.0 . . . . ?
Cs Nd O4 Sr 0.0 97_666 . . . ?
O3 Nd O4 Sr 0.0 148_565 . . . ?
O3 Nd O4 Sr 0.0 52 . . . ?
O3 Nd O4 Sr 0.0 147_556 . . . ?
O3 Nd O4 Sr 0.0 51_564 . . . ?
O3 Nd O4 Sr 0.0 98_655 . . . ?
O3 Nd O4 Sr 0.0 2_566 . . . ?
O2 Nd O4 Sr 0.0 177_556 . . . ?
O2 Nd O4 Sr 0.0 81 . . . ?
O4 Nd O4 Ce 0.0 97_666 . . . ?
Cs Nd O4 Ce 0.0 . . . . ?
Cs Nd O4 Ce 0.0 97_666 . . . ?
O3 Nd O4 Ce 0.0 148_565 . . . ?
O3 Nd O4 Ce 0.0 52 . . . ?
O3 Nd O4 Ce 0.0 147_556 . . . ?
O3 Nd O4 Ce 0.0 51_564 . . . ?
O3 Nd O4 Ce 0.0 98_655 . . . ?
O3 Nd O4 Ce 0.0 2_566 . . . ?
O2 Nd O4 Ce 0.0 177_556 . . . ?
O2 Nd O4 Ce 0.0 81 . . . ?
O4 Nd O4 U 0.0 97_666 . . . ?
Cs Nd O4 U 0.0 . . . . ?
Cs Nd O4 U 0.0 97_666 . . . ?
O3 Nd O4 U 0.0 148_565 . . . ?
O3 Nd O4 U 0.0 52 . . . ?
O3 Nd O4 U 0.0 147_556 . . . ?
O3 Nd O4 U 0.0 51_564 . . . ?
O3 Nd O4 U 0.0 98_655 . . . ?
O3 Nd O4 U 0.0 2_566 . . . ?
O2 Nd O4 U 0.0 177_556 . . . ?
O2 Nd O4 U 0.0 81 . . . ?
O4 Nd O4 Bi 0.0 97_666 . . . ?
Cs Nd O4 Bi 0.0 . . . . ?
Cs Nd O4 Bi 0.0 97_666 . . . ?
O3 Nd O4 Bi 0.0 148_565 . . . ?
O3 Nd O4 Bi 0.0 52 . . . ?
O3 Nd O4 Bi 0.0 147_556 . . . ?
O3 Nd O4 Bi 0.0 51_564 . . . ?
O3 Nd O4 Bi 0.0 98_655 . . . ?
O3 Nd O4 Bi 0.0 2_566 . . . ?
O2 Nd O4 Bi 0.0 177_556 . . . ?
O2 Nd O4 Bi 0.0 81 . . . ?
O4 Nd O4 La 0.0 97_666 . . . ?
Cs Nd O4 La 0.0 . . . . ?
Cs Nd O4 La 0.0 97_666 . . . ?
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O3 Nd O4 La 0.0 148_565 . . . ?
O3 Nd O4 La 0.0 52 . . . ?
O3 Nd O4 La 0.0 147_556 . . . ?
O3 Nd O4 La 0.0 51_564 . . . ?
O3 Nd O4 La 0.0 98_655 . . . ?
O3 Nd O4 La 0.0 2_566 . . . ?
O2 Nd O4 La 0.0 177_556 . . . ?
O2 Nd O4 La 0.0 81 . . . ?
O4 Nd O4 Pb -120(100) 97_666 . . 4 ?
Cs Nd O4 Pb 0.0 . . . 4 ?
Cs Nd O4 Pb -120(100) 97_666 . . 4 ?
O3 Nd O4 Pb 180.0 148_565 . . 4 ?
O3 Nd O4 Pb 0.0 52 . . 4 ?
O3 Nd O4 Pb -60.0 147_556 . . 4 ?
O3 Nd O4 Pb 120.0 51_564 . . 4 ?
O3 Nd O4 Pb 60.0 98_655 . . 4 ?
O3 Nd O4 Pb -120.0 2_566 . . 4 ?
O2 Nd O4 Pb 120.0 177_556 . . 4 ?
O2 Nd O4 Pb -60.0 81 . . 4 ?
O4 Nd O4 Ca 0(100) 97_666 . . 26 ?
Cs Nd O4 Ca 0.0 . . . 26 ?
Cs Nd O4 Ca 0(100) 97_666 . . 26 ?
O3 Nd O4 Ca -60.0 148_565 . . 26 ?
O3 Nd O4 Ca 120.0 52 . . 26 ?
O3 Nd O4 Ca 60.0 147_556 . . 26 ?
O3 Nd O4 Ca -120.0 51_564 . . 26 ?
O3 Nd O4 Ca 180.0 98_655 . . 26 ?
O3 Nd O4 Ca 0.0 2_566 . . 26 ?
O2 Nd O4 Ca -120.0 177_556 . . 26 ?
O2 Nd O4 Ca 60.0 81 . . 26 ?
O4 La O4 Pb 0.0 97_666 . . . ?
Cs La O4 Pb 0.0 . . . . ?
Cs La O4 Pb 0.0 97_666 . . . ?
O3 La O4 Pb 0.0 148_565 . . . ?
O3 La O4 Pb 0.0 52 . . . ?
O3 La O4 Pb 0.0 147_556 . . . ?
O3 La O4 Pb 0.0 51_564 . . . ?
O3 La O4 Pb 0.0 98_655 . . . ?
O3 La O4 Pb 0.0 2_566 . . . ?
O2 La O4 Pb 0.0 177_556 . . . ?
O2 La O4 Pb 0.0 81 . . . ?
O4 La O4 Ca 0.0 97_666 . . . ?
Cs La O4 Ca 0.0 . . . . ?
Cs La O4 Ca 0.0 97_666 . . . ?
O3 La O4 Ca 0.0 148_565 . . . ?
O3 La O4 Ca 0.0 52 . . . ?
O3 La O4 Ca 0.0 147_556 . . . ?
O3 La O4 Ca 0.0 51_564 . . . ?
O3 La O4 Ca 0.0 98_655 . . . ?
O3 La O4 Ca 0.0 2_566 . . . ?
O2 La O4 Ca 0.0 177_556 . . . ?
O2 La O4 Ca 0.0 81 . . . ?
O4 La O4 Mn 0.0 97_666 . . . ?
Cs La O4 Mn 0.0 . . . . ?
Cs La O4 Mn 0.0 97_666 . . . ?
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O3 La O4 Mn 0.0 148_565 . . . ?
O3 La O4 Mn 0.0 52 . . . ?
O3 La O4 Mn 0.0 147_556 . . . ?
O3 La O4 Mn 0.0 51_564 . . . ?
O3 La O4 Mn 0.0 98_655 . . . ?
O3 La O4 Mn 0.0 2_566 . . . ?
O2 La O4 Mn 0.0 177_556 . . . ?
O2 La O4 Mn 0.0 81 . . . ?
O4 La O4 Ba 0.0 97_666 . . . ?
Cs La O4 Ba 0.0 . . . . ?
Cs La O4 Ba 0.0 97_666 . . . ?
O3 La O4 Ba 0.0 148_565 . . . ?
O3 La O4 Ba 0.0 52 . . . ?
O3 La O4 Ba 0.0 147_556 . . . ?
O3 La O4 Ba 0.0 51_564 . . . ?
O3 La O4 Ba 0.0 98_655 . . . ?
O3 La O4 Ba 0.0 2_566 . . . ?
O2 La O4 Ba 0.0 177_556 . . . ?
O2 La O4 Ba 0.0 81 . . . ?
O4 La O4 Sr 0.0 97_666 . . . ?
Cs La O4 Sr 0.0 . . . . ?
Cs La O4 Sr 0.0 97_666 . . . ?
O3 La O4 Sr 0.0 148_565 . . . ?
O3 La O4 Sr 0.0 52 . . . ?
O3 La O4 Sr 0.0 147_556 . . . ?
O3 La O4 Sr 0.0 51_564 . . . ?
O3 La O4 Sr 0.0 98_655 . . . ?
O3 La O4 Sr 0.0 2_566 . . . ?
O2 La O4 Sr 0.0 177_556 . . . ?
O2 La O4 Sr 0.0 81 . . . ?
O4 La O4 Ce 0.0 97_666 . . . ?
Cs La O4 Ce 0.0 . . . . ?
Cs La O4 Ce 0.0 97_666 . . . ?
O3 La O4 Ce 0.0 148_565 . . . ?
O3 La O4 Ce 0.0 52 . . . ?
O3 La O4 Ce 0.0 147_556 . . . ?
O3 La O4 Ce 0.0 51_564 . . . ?
O3 La O4 Ce 0.0 98_655 . . . ?
O3 La O4 Ce 0.0 2_566 . . . ?
O2 La O4 Ce 0.0 177_556 . . . ?
O2 La O4 Ce 0.0 81 . . . ?
O4 La O4 U 0.0 97_666 . . . ?
Cs La O4 U 0.0 . . . . ?
Cs La O4 U 0.0 97_666 . . . ?
O3 La O4 U 0.0 148_565 . . . ?
O3 La O4 U 0.0 52 . . . ?
O3 La O4 U 0.0 147_556 . . . ?
O3 La O4 U 0.0 51_564 . . . ?
O3 La O4 U 0.0 98_655 . . . ?
O3 La O4 U 0.0 2_566 . . . ?
O2 La O4 U 0.0 177_556 . . . ?
O2 La O4 U 0.0 81 . . . ?
O4 La O4 Bi 0.0 97_666 . . . ?
Cs La O4 Bi 0.0 . . . . ?
Cs La O4 Bi 0.0 97_666 . . . ?
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O3 La O4 Bi 0.0 148_565 . . . ?
O3 La O4 Bi 0.0 52 . . . ?
O3 La O4 Bi 0.0 147_556 . . . ?
O3 La O4 Bi 0.0 51_564 . . . ?
O3 La O4 Bi 0.0 98_655 . . . ?
O3 La O4 Bi 0.0 2_566 . . . ?
O2 La O4 Bi 0.0 177_556 . . . ?
O2 La O4 Bi 0.0 81 . . . ?
O4 La O4 Nd 0.0 97_666 . . . ?
Cs La O4 Nd 0.0 . . . . ?
Cs La O4 Nd 0.0 97_666 . . . ?
O3 La O4 Nd 0.0 148_565 . . . ?
O3 La O4 Nd 0.0 52 . . . ?
O3 La O4 Nd 0.0 147_556 . . . ?
O3 La O4 Nd 0.0 51_564 . . . ?
O3 La O4 Nd 0.0 98_655 . . . ?
O3 La O4 Nd 0.0 2_566 . . . ?
O2 La O4 Nd 0.0 177_556 . . . ?
O2 La O4 Nd 0.0 81 . . . ?
O4 La O4 Pb -120(100) 97_666 . . 4 ?
Cs La O4 Pb 0.0 . . . 4 ?
Cs La O4 Pb -120(100) 97_666 . . 4 ?
O3 La O4 Pb 180.0 148_565 . . 4 ?
O3 La O4 Pb 0.0 52 . . 4 ?
O3 La O4 Pb -60.0 147_556 . . 4 ?
O3 La O4 Pb 120.0 51_564 . . 4 ?
O3 La O4 Pb 60.0 98_655 . . 4 ?
O3 La O4 Pb -120.0 2_566 . . 4 ?
O2 La O4 Pb 120.0 177_556 . . 4 ?
O2 La O4 Pb -60.0 81 . . 4 ?
O4 La O4 Ca 0(100) 97_666 . . 26 ?
Cs La O4 Ca 0.0 . . . 26 ?
Cs La O4 Ca 0(100) 97_666 . . 26 ?
O3 La O4 Ca -60.0 148_565 . . 26 ?
O3 La O4 Ca 120.0 52 . . 26 ?
O3 La O4 Ca 60.0 147_556 . . 26 ?
O3 La O4 Ca -120.0 51_564 . . 26 ?
O3 La O4 Ca 180.0 98_655 . . 26 ?
O3 La O4 Ca 0.0 2_566 . . 26 ?
O2 La O4 Ca -120.0 177_556 . . 26 ?
O2 La O4 Ca 60.0 81 . . 26 ?
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