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THE CRYSTAL STRUCTURE OF SCHUILINGITE-(Nd)

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ABSTRACT

Schuilingite-(Nd) from the Kasompi copper mine, Katanga, southern Shaba, Democratic Republic of Congo, crystallizes in the space group $P2_1cn$, with a 7.419(2), b 18.859(3), c 6.395(1) Å, V 894.7(3) Å^3, Z = 4. The structure of schuilingite-(Nd), Pb^{2+} Cu^{2+} (*REE*) $(CO_3)_3$ (OH) (H_2O), has one site occupied by rare-earth elements, *REE* (predominantly Nd) and coordinated by nine O atoms and one (OH) group. There is one *Pb* site occupied by Pb^{2+} coordinated by seven O atoms and one (OH) group in a very asymmetric arrangement that is characteristic of stereoactive lone-pair-electron behavior of Pb^{2+}. There is one *Cu* site occupied by Cu^{2+} coordinated by three O atoms, one (OH) group and one (H_2O) group in a square-pyramidal arrangement. The structure contains chains of face-sharing $(REE\phi_{10})$ polyhedra that link to chains of $(Cu\phi_5)$ and $(Pb\phi_7)$ polyhedra by sharing edges and corners and through (CO_3) groups. Schuilingite-(Nd) is structurally related to gysinite-(Nd), another Nd-dominant *REE* carbonate mineral. The structure of gysinite-(Nd) also contains chains of face-sharing $(REE\phi_{10})$ polyhedra linked in a fashion similar to the analogous chains in schuilingite-(Nd). The space-group symmetry of gysinite-(Nd) is *Pmcn*, a supergroup of $P2_1cn$. Loss of the center of symmetry in schuilingite-(Nd) is related to replacement of every second chain of $(REE\phi_{10})$ polyhedra by two $(Cu\phi_5)$–$(Pb\phi_7)$ chains of polyhedra.

Keywords: schuilingite-(Nd), crystal structure, carbonate, rare-earth element, gysinite-(Nd).

SOMMAIRE

La schuilingite-(Nd) de la mine de cuivre de Kasompi, au Katanga, dans le sud de la province de Shaba, République Démocratique du Congo, cristallise dans le groupe spatial $P2_1cn$, avec a 7.419(2), b 18.859(3), c 6.395(1) Å, V 894.7(3) Å^3, Z = 4. La structure de la schuilingite-(Nd), Pb^{2+} Cu^{2+} (*TR*) $(CO_3)_3$ (OH) (H_2O), possède un site qu'occupent les terres rares, *TR* (surtout Nd), à coordinence dix, avec neuf atomes d'oxygène et un groupe (OH). Il y a un site *Pb*; l'ion Pb^{2+} est en coordinence avec sept atomes d'oxygène et un groupe (OH). La répartition de ces liaisons est fortement assymétrique, caractéristique d'un comportement d'une paire isolée d'électrons stéréoactifs de l'ion Pb^{2+}. Il y a un site *Cu* qu'occupe le Cu^{2+} en coordinence avec trois atomes d'oxygène, un groupe (OH) et un groupe (H_2O) dans un agencement en pyramide carrée. La structure contient des chaînes de polyèdres $(REE\phi_{10})$ à faces partagées qui sont rattachées à des chaînes de polyèdres $(Cu\phi_5)$ et $(Pb\phi_7)$ par partage d'arêtes et de coins, et par le biais des groupes (CO_3). La structure de la schuilingite-(Nd) montre des points communs avec celle de la gysinite-(Nd), un autre minéral carbonaté à dominance de Nd. La gysinite-(Nd) contient aussi des chaînes de polyèdres $(TR\phi_{10})$ à faces partagées, tout comme la schuilingite-(Nd). Le groupe spatial de la gysinite-(Nd) est *Pmcn*, un supergroupe de $P2_1cn$. La perte d'un centre de symétrie dans la schuilingite-(Nd) relève du remplacement de chaque deuxième chaîne de polyèdres $(TR\phi_{10})$ par deux chaînes de polyèdres $(Cu\phi_5)$–$(Pb\phi_7)$.

(Traduit par la Rédaction)

Mots-clés: schuilingite-(Nd), structure cristalline, carbonate, terre rare, gysinite-(Nd).

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INTRODUCTION

Schuilingite-(Nd) was first described by Vaes (1947) as a Cu–Pb mineral. Guillemin & Pierrot (1957) characterized schuilingite-(Nd) as a Ca–Pb–Cu carbonate, and they gave information on physical properties and mineral associations, together with an unindexed X-ray powder pattern. Piret & Deliens (1982) reported that schuilingite-(Nd) has the general formula Pb Cu *REE* $(CO_3)_3$ (OH) $(H_2O)_{1.5}$ with *REE* = $Y_{0.118}La_{0.040}Pr_{0.045}Nd_{0.329}Sm_{0.128}Eu_{0.091}Gd_{0.142}Dy_{0.107}$. Their chemical analyses show large variations in the proportions of the rare-earth elements (*REE*). Indexing of the powder-diffraction pattern gave space-group symmetry $P2_1cn$ with *a* 7.418, *b* 18.87 and *c* 6.385 Å. Schuilingite-(Nd) occurs in the weathering zone of the copper deposits at Menda and Kasompi, southern Shaba, Democratic Republic of Congo. In this paper, we report the structure of schuilingite-(Nd) and examine its structural relation with gysinite-(Nd).

EXPERIMENTAL

Sample

The material is from Kasompi, Katanga, southern Shaba, Democratic Republic of Congo, and contains complex intergrowths of bright blue crystals of schuilingite-(Nd) in association with gysinite-(Nd).

Collection of X-ray diffraction data

A crystal was mounted on a Nicolet *R*3*m* automated four-circle diffractometer. Thirty-six reflections were centered using graphite-monochromatized MoKα X-radiation; the resulting unit-cell dimensions are given in Table 1. A total of 2739 symmetry-independent reflections was measured ($4 \leq 2\theta \leq 60°$), with index ranges $0 \leq h \leq 10$, $0 \leq k \leq 26$, $-9 \leq l \leq 9$ and with a fixed scan speed of 0.8°2θ/min. Two standard reflections were measured every fifty-eight reflections; there were no significant changes in their intensities during data collection. An empirical absorption-correction based on 36 psi-scans of each of nine reflections was applied, with the crystal modeled as an ellipsoid. The absorption correction reduced *R* (*azimuthal*) from 6.5 to 1.5%. The intensity data were corrected for Lorentz, polarization and background effects, and reduced to structure factors. A reflection was considered as observed if its structure factor exceeded that of five standard deviations above background, based on counting statistics.

TABLE 1. EXPERIMENTAL DATA FOR SCHUILINGITE-(Nd)

Crystal system	orthorhombic	Crystal size (μm)	25 x 25 x 60
Space group	$P2_1cn$	Wavelength (Å)	MoKα
a (Å)	7.419(2)	μm (mm^{-1})	26.9
b (Å)	18.859(3)	No. of I	2739
c (Å)	6.395(1)	No. of unique |*F*|	1400
V ($Å^3$)	894.7(3)	No. of $\|F_{obs}\| > 5\sigma F$	1094
Z	4	R_{int} (%)	0.7
R (%)	3.8	$R = \Sigma(\|F_o\|-\|F_c\|)/\Sigma\|F_o\|$	
wR (%)	4.6	$wR = [\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma F_o^2]^{1/2}$, $w = 1$	

Refinement of the crystal structure

Scattering curves for neutral atoms, together with anomalous-dispersion corrections, were taken from Cromer & Mann (1968) and Cromer & Liberman (1970), respectively. The SHELXL system of programs (Sheldrick 1990) was used for this work.

The structure was solved and refined in the space group $P2_1cn$. During refinement, the anisotropic-displacement factors for O and C became non-positive definite; thus, these atoms were refined isotropically. The final cycles of refinement involved all variable positional parameters, anisotropic- and isotropic-displacement factors. The structure converged to an *R*-index of 3.8%. Final atom positions and isotropic- or equivalent-isotropic-displacement factors are listed in Table 2. Selected interatomic distances and angles were calculated with SADIAN90 (Baur & Kassner 1991) and are shown in Table 3; a bond-valence table is shown as Table 4. Structure factors may be obtained from the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada.

TABLE 2. POSITIONAL COORDINATES AND ISOTROPIC-DISPLACEMENT PARAMETERS FOR SCHUILINGITE-(Nd)

	x	*y*	*z*	U_{iso} (x 10^3)
Pb	½	0.86016(3)	0.3820(1)	15.8(2)*
Nd	0.0011(5)	0.69205(4)	0.1020(1)	9.6(3)*
Cu	0.2934(6)	0.5587(2)	0.3115(4)	16.6(8)*
C(1)	0.159(3)	0.840(1)	0.108(4)	18(3)
C(2)	0.670(3)	0.783(1)	0.823(4)	15(4)
C(3)	−0.067(3)	0.542(1)	0.012(4)	13(4)
O(1)	0.251(3)	0.8955(9)	0.082(3)	18(3)
O(2)	0.047(2)	0.8172(8)	−0.026(3)	17(3)
O(3)	0.186(3)	0.8038(9)	0.276(2)	18(3)
O(4)	0.697(3)	0.8401(9)	0.720(3)	14(4)
O(5)	0.523(4)	0.7720(7)	0.919(2)	20(4)
O(6)	0.796(3)	0.7346(8)	0.819(3)	15(3)
O(7)	0.008(5)	0.5539(8)	0.191(2)	23(3)
O(8)	−0.095(3)	0.5944(9)	−0.115(3)	21(4)
O(9)	−0.098(3)	0.477(1)	−0.051(3)	27(4)
O(10)	0.304(3)	0.6517(9)	0.166(3)	12(3)
O(11)	0.294(3)	0.033(1)	0.955(3)	28(4)

* equivalent isotropic-displacement parameter

TABLE 3. SELECTED INTERATOMIC DISTANCES [Å] AND ANGLES [°] IN SCHUILINGITE-(Nd)

Pb–O(10)a	2.34(2)	*Nd*–O(10)	2.41(2)
Pb–O(5)a	2.51(1)	*Nd*–O(2)a	2.41(2)
Pb–O(9)c	2.56(2)	*Nd*–O(8)	2.41(2)
Pb–O(4)	2.64(2)	*Nd*–O(4)a	2.46(2)
Pb–O(3)	2.65(2)	*Nd*–O(6)b	2.48(2)
Pb–O(1)	2.75(2)	*Nd*–O(3)a	2.50(2)
Pb–O(6)b	2.86(2)	*Nd*–O(6)a	2.50(2)
Pb–O(8)	3.13(2)	*Nd*–O(2)	2.52(2)
<*Pb*–O>	2.68(2)	*Nd*–O(7)	2.67(2)
		Nd–O(3)	2.75(2)
Cu–O(11)a	1.96(2)	<*Nd*–O>	2.51(2)
Cu–O(1)a	1.96(2)		
Cu–O(9)a	1.97(2)	O(11)–O(8)	2.60(3)
Cu–O(10)	1.99(2)	O(11)–O(7)	2.79(3)
Cu–O(7)	2.26(3)		
<*Cu*–O>	2.03(2)	O(1)–C(1)–O(2)	123(2)
		O(1)–C(1)–O(3)	117(2)
C(1)–O(1)	1.26(3)	O(2)–C(1)–O(3)	119(2)
C(1)–O(2)	1.27(3)		
C(1)–O(3)	1.29(3)	O(4)–C(2)–O(5)	122(2)
<C(1)–O>	1.27(3)	O(4)–C(2)–O(6)	118(2)
		O(5)–C(2)–O(6)	121(2)
C(2)–O(4)	1.27(3)		
C(2)–O(5)	1.28(3)	O(7)–C(3)–O(8)	120(2)
C(2)–O(6)	1.31(3)	O(7)–C(3)–O(9)	121(2)
<C(2)–O>	1.29(3)	O(8)–C(3)–O(9)	120(2)
C(3)–O(7)	1.29(3)	O(8)–O(11)–O(7)	115(2)
C(3)–O(8)	1.30(3)	O(10)–O(5)	2.71(3)
C(3)–O(9)	1.31(3)		
<C(3)–O>	1.30(2)		

a = *x*, 1½–*y*, ½–*z*; b = –*x*, 1½–*y*, ½–*z*; c = ½–*x*, ½+*y*, ½–*z*

Electron-microprobe analysis

We had great trouble finding a crystal suitable for collection of X-ray intensity data, and were unwilling to sacrifice it to the electron microprobe. Thus five crystals of the same sample were mounted and carbon-coated for chemical analysis with a Cameca SX–50 electron microprobe operating in the wavelength-dispersion mode with an excitation voltage of 15 kV, a specimen current of 10 nA and a beam size of 20 μm. The following standards were used: azurite (Cu), *REE* glasses (Drake & Weill 1972) and PbTe. Data reduction was done according to the ϕρz method (Pouchou & Pichoir 1984, 1985), and the average chemical composition of five crystals (19 points) is given in Table 5. The unit formula was calculated on the basis of 11 anions, assuming stoichiometric C and H.

CRYSTAL STRUCTURE

The Nd site

There is one site containing the *REE*; this was designated the *Nd* site. The site-scattering value of the *Nd* site was refined using the scattering curve for neutral Nd, and converged to a value of 59.5(4) *epfu* (electrons per formula unit). This value is in close agreement with the value of 59.1 *epfu* calculated from the average composition determined by electron-microprobe analysis (Table 5). The average chemical formula for all five schuilingite-(Nd) crystals can be written as $Pb_{1.05}$ $Cu_{0.92}$ $(REE)_{1.02}$ $(CO_3)_3$ (OH) (H_2O) with *REE* = $Y_{0.16}$ $La_{0.04}$ $Pr_{0.03}$ $Nd_{0.24}$ $Sm_{0.12}$ $Eu_{0.06}$ $Gd_{0.18}$ $Tb_{0.02}$ $Dy_{0.13}$ $Er_{0.03}$ $Yb_{0.01}$. The average chemical composition of each crystal shows clearly the dominance of Nd, followed by Gd and Y. The *Nd* site is in [10]-coordination, and the mean

TABLE 4. BOND-VALENCE* (*vu*) TABLE FOR SCHUILINGITE-(Nd)

	Pb	*Nd*	*Cu*	C(1)	C(2)	C(3)	*H*(1)	*H*(2)	*H*(3)	Σ
O(1)	0.20		0.47	1.42						2.09
O(2)		0.40 0.31		1.38						2.09
O(3)	0.24	0.33 0.16		1.31						2.04
O(4)	0.25	0.36			1.38					1.99
O(5)	0.32				1.35				0.20	1.87
O(6)	0.16	0.33 0.31			1.24					2.04
O(7)		0.21	0.21			1.31	0.20			1.93
O(8)	0.10	0.39				1.28		0.20		1.97
O(9)	0.29		0.46			1.24				1.99
O(10)	0.48	0.40	0.43						0.80	2.11
O(11)			0.47				0.80	0.80		2.07
Σ	2.04	3.20	2.04	4.11	3.97	3.83	1.00	1.00	1.00	

*The bond-valence curves are from Brown (1981) and Brown & Altermatt (1985).

TABLE 5. CHEMICAL COMPOSITIONS OF FIVE SCHUILINGITE-(Nd) CRYSTALS

	No. 1 (n=5)	No. 2 (n=5)	No. 3 (n=3)	No. 4 (n=4)	No. 5 (n=3)	Aver. (n=19)
PbO	36.25	35.85	36.84	36.78	36.26	36.85
CuO	11.43	11.20	11.51	11.19	11.53	11.35
Y_2O_3	2.87	2.64	2.57	3.10	3.44	2.90
La_2O_3	0.91	0.98	1.16	0.91	0.78	0.94
Pr_2O_3	0.90	0.89	0.71	0.74	0.63	0.80
Nd_2O_3	6.42	7.17	6.41	5.76	5.32	6.31
Sm_2O_3	3.18	3.57	3.15	3.03	2.65	3.16
Eu_2O_3	1.54	1.75	1.73	1.58	1.53	1.63
Gd_2O_3	5.12	4.99	5.08	5.19	5.29	5.12
Tb_2O_3	0.51	0.70	0.70	0.68	0.77	0.66
Dy_2O_3	3.66	3.38	3.50	4.14	4.21	3.74
Er_2O_3	0.85	0.80	0.71	1.09	1.02	0.89
Yb_2O_3	0.15	0.36	0.33	0.40	0.29	0.30
H_2O^*	4.19	4.22	4.20	4.22	4.20	4.20
CO_2^*	20.47	20.61	20.52	20.60	20.50	20.54
Total	98.48	99.11	99.12	99.40	98.42	98.91
Pb^{2+}	1.05	1.03	1.06	1.06	1.05	1.05
Cu^{2+}	0.93	0.90	0.93	0.90	0.93	0.92
Y^{3+}	0.16	0.15	0.15	0.17	0.20	0.16
La^{3+}	0.04	0.04	0.05	0.04	0.03	0.04
Pr^{3+}	0.04	0.04	0.03	0.03	0.03	0.03
Nd^{3+}	0.25	0.27	0.25	0.22	0.20	0.24
Sm^{3+}	0.12	0.13	0.12	0.11	0.10	0.12
Eu^{3+}	0.06	0.06	0.06	0.06	0.06	0.06
Gd^{3+}	0.18	0.18	0.18	0.18	0.15	0.18
Tb^{3+}	0.02	0.02	0.03	0.02	0.03	0.02
Dy^{3+}	0.13	0.12	0.12	0.14	0.15	0.13
Er^{3+}	0.03	0.03	0.02	0.04	0.03	0.03
Yb^{3+}	0.01	0.01	0.01	0.01	0.01	0.01
H^+	3.0	3.0	3.0	3.0	3.0	3.0
C^{4+} *	3.0	3.0	3.0	3.0	3.0	3.0

* determined by stoichiometry; Ce not detected

Nd–O bond length is 2.51 Å (Table 2). The incident bond-valence sum at the *Nd* site is 3.2 *vu* (valence units) (Table 4), on the basis of the average chemical composition of the grains analyzed.

The Cu site

There is one *Cu* site, with a site-scattering value in accord with occupancy of this site by Cu; the stereochemistry around the *Cu* site and the sum of the bond valences incident at this site (Table 4) indicate that Cu is in the divalent state. The *Cu* site has elongate square-pyramidal coordination; there are four similar equatorial *Cu*–O bonds with an average value of <2.03 Å> and one longer apical bond of 2.26 Å (Table 3).

Eby & Hawthorne (1990) reported sixteen Cu^{2+}-oxysalt minerals containing Cu^{2+} in [5]-coordination. They showed that Cu^{2+} in minerals occurs more commonly in square-pyramidal than in triangular-bipyramidal coordination, despite the fact that the triangular-bipyramidal coordination is energetically favored over the square-pyramidal coordination (Burns 1994) . The structure of schuilingite-(Nd) is one further example of the occurrence of elongate square-pyramidal coordination. Reinen & Atanasov (1989) have argued that vibronic interaction between the ground state and the excited state leads to stabilization of the elongate square-pyramid over the triangular bipyramid as the excited state is Jahn–Teller active.

The Pb site

The *Pb* site is coordinated by eight O atoms (Fig. 1). There are seven *Pb*–O distances between 2.33 and 2.85 Å with an average *Pb*–O distance of <2.62 Å>, and there is one *Pb*–O distance of 3.13 Å. The latter *Pb*–O distance is quite long, and it is not clear from the bond-valence value whether or not it should be considered a bond (Table 4). However, what is clear from Figure 1 is that the coordination of Pb^{2+} is very asymmetrical: the six shortest bonds are on one side of the central cation, and the two longest bonds, *Pb*–O(6) and *Pb*–O(8), are on the other side of the cation (Fig. 1). This type of coordination geometry is characteristic of stereoactive lone-pair behavior by the central cation.

Hydrogen bonding

No H positions were located in the final difference-Fourier map, and OH and H_2O groups were assigned on the basis of bond-valence requirements (Table 4). The equatorial O atom [O(11)] of the square pyramid bonds only to Cu^{2+} and receives a bond valence of 0.48 *vu* from this cation. In order to satisfy its incident bond-valence requirement , the O(11) site must be occupied by an H_2O group. In the same way, the equatorial O(10) site is assigned as an (OH) group, receiving an incident bond-valence of 1.32 *vu* from Pb^{2+}, Nd^{3+} and Cu^{2+} (Table 4). The H bonds involving the H_2O group (Figs. 2, 3) link to O(7) and O(8), which are located on the opposite side of the seven-membered ring. The hydrogen bond from the OH-group [O(10)] links to O(5) (Figs. 2, 3 and 4).

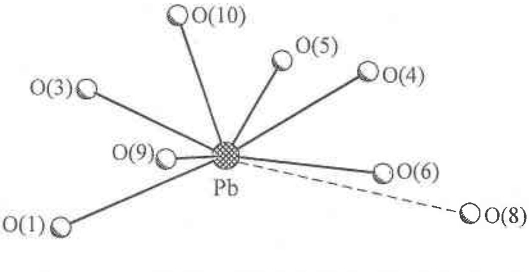

FIG. 1. The coordination of the *Pb* site in schuilingite-(Nd).

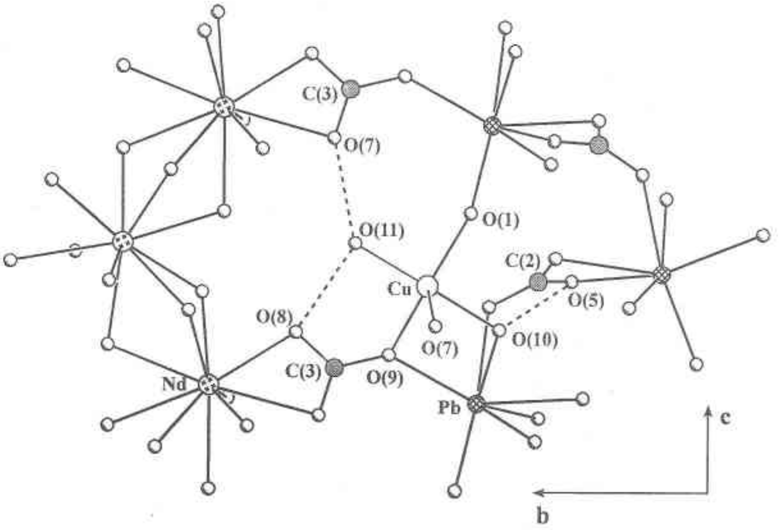

FIG. 2. The H bonding in schuilingite-(Nd); H bonds are shown as broken lines.

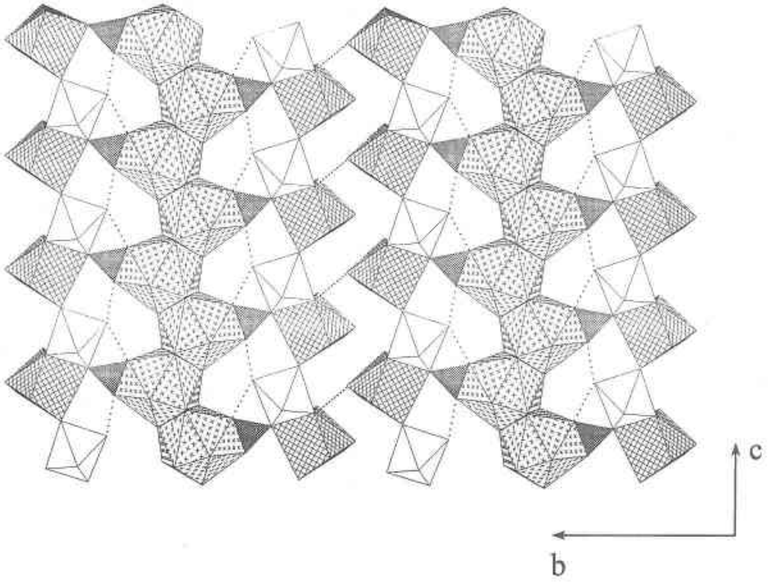

FIG. 3. Part of the schuilingite-(Nd) structure parallel the *a* axis: the face-shared ($Nd\phi_{10}$) polyhedra are cross-shaded, the ($Pb\phi_7$) polyhedra are shaded with a 4^4 net, and the ($Cu\phi_5$) pyramids are blank. The H bonds are shown as dotted lines.

Structure topology

Figure 3 shows the characteristic features of the schuilingite-(Nd) structure. The ($Nd\phi_{10}$) polyhedra (ϕ: undefined ligand) share faces to form kinked chains that extend parallel to the *c* axis. The ($Pb\phi_7$) and ($Cu\phi_5$) polyhedra share an edge to form a pair, and these pairs link together by sharing corners to form chains that also extend parallel to the *c* axis (Fig. 3). These two types of chains link by sharing edges between the ($Nd\phi_{10}$) and

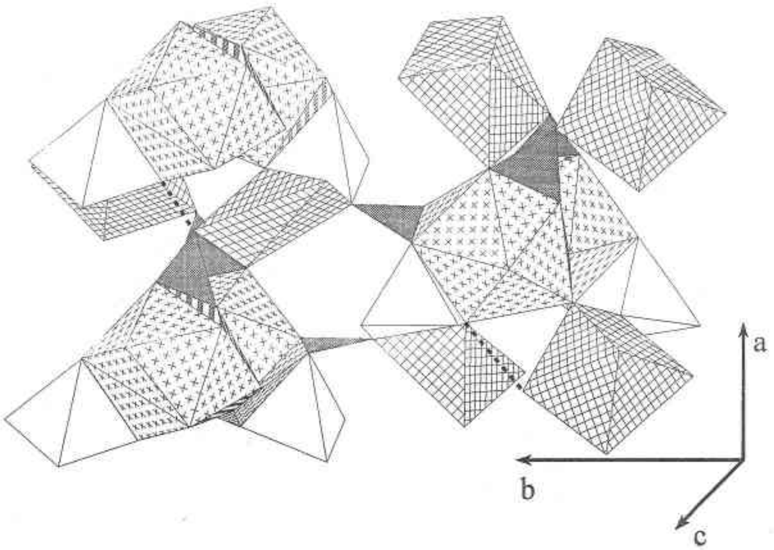

FIG. 4. Part of the schuilingite-(Nd) structure parallel to the c axis: the face-shared $(Nd\phi_{10})$ polyhedra alternate in the a direction with chains of $(Pb\phi_7)$ polyhedra and $(Cu\phi_5)$ pyramids; legend as in Figure 3.

$(Cu\phi_5)$ polyhedra (Fig. 4) and corners between all polyhedra. Carbonate groups link the chains in the [010] direction (Fig. 3). This kind of arrangement produces seven-membered rings with the sequence of central cations Nd–Nd–Nd–C–Cu–Pb–C. These seven-membered rings in the *bc* plane produce a system of channels parallel to the *a* axis, and the H_2O groups are located in these channels. Each plane shown in Figure 3 is symmetrically related to adjacent planes by two-fold screw axes through the channels parallel to *a* (Fig. 5). The hydrogen bond of the OH group bridges two parallel $(Cu\phi_5)$–$(Pb\phi_7)$ chains (Figs. 2, 3 and 4).

Relations to gysinite-(Nd) and other carbonates

The structure of gysinite-(Nd), $(Nd_{1.18}Pb_{0.66}La_{0.16})_{\Sigma 2.00}(CO_3)_2(OH)_{1.34}(H_2O)_{0.66}$, has space-group symmetry *Pmcn* (Chabot & Sarp 1985), and like schuilingite-(Nd), it contains face-sharing $(REE,Pb\phi_{10})$ polyhedra in chains parallel to the *c* axis. Gysinite-(Nd) is isotypic with ancylite, $(REE)_x(Ca, Sr)_{2-x}(CO_3)_2(OH)_x(H_2O)_{2-x}$ (Dal Negro *et al.* 1975), and is related to the orthorhombic carbonates aragonite, strontianite and witherite. In the latter structures, the alkaline-earth cations are coordinated by nine O atoms, whereas in ancylite and gysinite-(Nd), the *REE* cations are coordinated by nine O atoms and one OH group. The space-group symmetry of gysinite-(Nd) and aragonite is *Pmcn*, a supergroup of $P2_1cn$ with [t] = 2 ([t] = *translationgleich*). Figure 5 shows the arrangements of the schuilingite-(Nd) and gysinite-(Nd) structures parallel to the *c* axis. The $(Nd\phi_{10})$ polyhedron in gysinite-(Nd) is symmetrically arranged along the mirror plane. In schuilingite-(Nd), every second $(Nd\phi_{10})$ polyhedron is replaced by two $(Cu\phi_5)$ square pyramids and two $(Pb\phi_7)$ polyhedra with stereoactive Pb^{2+} (Fig. 4). This replacement requires a different orientation of the carbonate group that links the $(Cu\phi_5)$–$(Pb\phi_7)$ polyhedron chain with the $(Nd\phi_{10})$ polyhedron chain in the *b* direction. Replacement of every second $(Nd\phi_{10})$ polyhedron by two $(Cu\phi_5)$–$(Pb\phi_7)$ dimers and the different orientation of the carbonate groups cause the loss of mirror symmetry perpendicular to *a* in schuilingite-(Nd). Thus, the lack of a center of symmetry in schuilingite-(Nd) is caused by replacement of every second chain of $(Nd\phi_{10})$ polyhedra by two chains of $(Cu\phi_5)$–$(Pb\phi_7)$ polyhedra. This replacement also causes a doubling of the *b* repeat and a shift of the structure ¼ along *c*.

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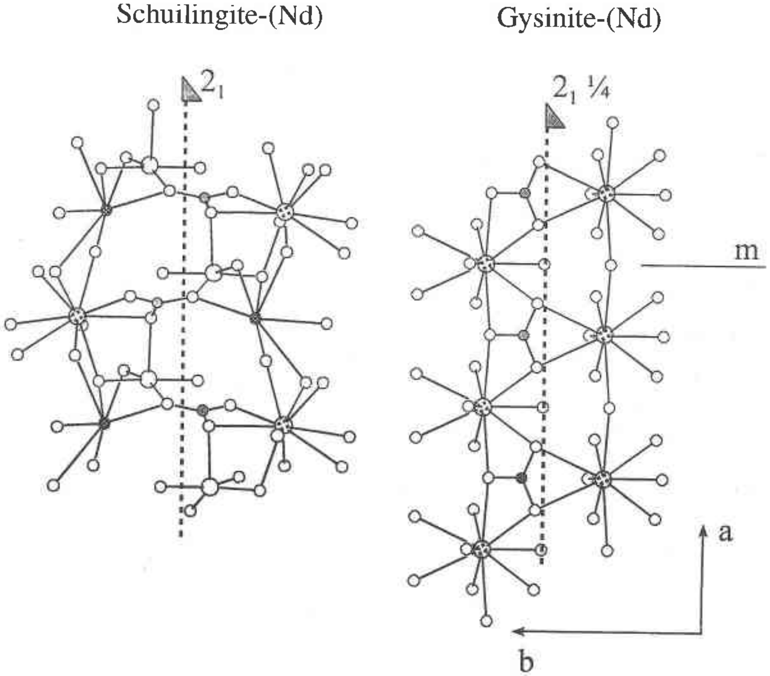

FIG. 5. Comparison of the structures of schuilingite-(Nd) and gysinite-(Nd) in the *ab* plane; legend as in Figure 2.

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