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THE CRYSTAL STRUCTURE OF RAPIDCREEKITE, $Ca_2(SO_4)(CO_3)(H_2O)_4$, AND ITS RELATION TO THE STRUCTURE OF GYPSUM

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ABSTRACT

The crystal structure of rapidcreekite, $Ca_2(SO_4)(CO_3)(H_2O)_4$, *a* 15.517(2), *b* 19.226(3), *c* 6.1646(8) Å, *V* 1839.0(4) Å^3, *Pcnb*, *Z* = 8, has been solved by direct methods and refined to an *R* index of 4.4% based on 943 observed (5σ) reflections measured with Mo*K*α X-radiation. There are two unique *Ca* sites, both of which are coordinated by six oxygen anions and two (H_2O) groups in a square antiprism arrangement. There is one unique *S* site coordinated by a tetrahedron of oxygen anions, and one *C* site coordinated by a triangle of oxygen anions. ($Ca\phi_8$) polyhedra share edges to form chains along [001] that are cross-linked in the [010] direction into a sheet by (CO_3) triangles and (SO_4) tetrahedra; the resulting sheet is the structural unit of rapidcreekite. Inter-unit linkage is provided by an array of H-bonds involving the (H_2O) groups of the sheet; this weak interstitial bonding accounts for the perfect {100} cleavage of rapidcreekite. The structure of rapidcreekite is related to the structure of gypsum by twinning of the gypsum structure along alternate rows of (SO_4) groups coupled with incorporation of (CO_3) groups along each twin plane.

Keywords: rapidcreekite, crystal structure, sulfate, carbonate, hydrogen bonding.

SOMMAIRE

Nous avons affiné la structure cristalline de la rapidcreekite, $Ca_2(SO_4)(CO_3)(H_2O)_4$, *a* 15.517(2), *b* 19.226(3), *c* 6.1646(8) Å, *V* 1839.0(4) Å^3, *Pcnb*, *Z* = 8, par méthodes directes jusqu'à un résidu *R* de 4.4% en utilisant 943 réflexions observées (5σ) et mesurées avec un rayonnement Mo*K*α. La structure contient deux positions distinctes occupées par le calcium, dans les deux cas en coordinence avec six atomes d'oxygène et deux groupes H_2O agencés en antiprisme carré. Les atomes de soufre occupent une seule position à coordinence tétraédrique avec quatre atomes d'oxygène, et les atomes de carbone sont entourés par trois atomes d'oxygène en arrangement triangulaire. Les polyèdres ($Ca\phi_8$) partagent des arêtes pour former des chaînes le long de [001], interconnectées dans la direction [010] par triangles (CO_3) et tétraèdres (SO_4) pour former des feuillets qui sont l'unité structurale de base. Les liens entre ces unités sont assurés par un réseau de liaisons hydrogène impliquant les groupes (H_2O) des feuillets; ces faibles liaisons interstitielles rendent compte du clivage {100} parfait. On peut relier la structure de la rapidcreekite à celle du gypse en maclant celle-ci le long de chaque deuxième rangée de groupes (SO_4) et en ajoutant des groupes (CO_3) le long de chaque plan de macle.

(Traduit par la Rédaction)

Mots-clés: rapidcreekite, structure cristalline, sulfate, carbonate, liaison hydrogène.

INTRODUCTION

Rapidcreekite, a hydrated calcium carbonate–sulfate, was described by Roberts *et al.* (1986) from a sequence of Lower Cretaceous (Albian) ironstones and shales in the Rapid Creek – Big Fish River area of the northern Yukon Territory. It occurs as a secondary phase on dilated joint-surfaces and bedding planes in a blocky quartz-rich bed in the sideritic iron-formation, and is associated with gypsum, aragonite and kulanite. Rapidcreekite occurs as radiating sprays of white to colorless acicular crystals, up to 2 mm long and 40 μm in diameter.

EXPERIMENTAL

The material on which the structure was solved is from Crosscut Creek, Rapid Creek area, Yukon Territory, and was purchased from a mineral dealer. Rapidcreekite diffracts extremely weakly and tends to give diffuse reflections owing to its occurrence as subparallel aggregates. The crystal used for the collection of the intensity data is a fiber, flattened on {010} and elongate along [001]. It was mounted on a Siemens *P4* automated four-circle diffractometer and oriented using all thirty-eight reflections (5 < 2θ < 25°) that could be detected on a long-exposure (70 min)

TABLE 1. MISCELLANEOUS INFORMATION FOR RAPIDCREEKITE

a (Å)	15.517(2)	Crystal size (μm)	44 x 26 x 140
b	19.226(3)	radiation	Mo$K\alpha$/Graphite
c	6.1646(8)	No. of intensities	2698
V (Å^3)	1839.0(4)	No. of $\lvert F_o\rvert > 5\sigma(\lvert F_o\rvert)$	943
Sp. Gr.	*Pcnb*	min. transmission	0.9388
Z	8	max. transmission	0.9672
mμ (mm^{-1})	1.52	R(obs) %	4.4
D$_c$ (g.cm^{-3})	2.227	wR(obs) %	4.6

Cell content: $8[Ca_2(SO_4)(CO_3)4H_2O]$

$R = \Sigma(\lvert F_o\rvert - \lvert F_c\rvert)/\Sigma\lvert F_o\rvert$

$wR = [\Sigma w(\lvert F_o\rvert - \lvert F_c\rvert)^2/\Sigma F_o^2]^{½}$, $w = 1/(\sigma^2 F + 0.00025F^2)$

rotation photograph with the generator at maximum power (55 kV, 50 mA). Refined cell-dimensions are given in Table 1. A total of 2698 unique reflections were collected over one asymmetric unit ($4 < 2\theta < 60°$; $\overline{21} \le h \le 0$, $0 \le k \le 27$, $\overline{8} \le l \le 0$) at a scan speed of 1.33° 2θ/min. Two check reflections were monitored every 50 reflections; there was no significant change in their diffracted intensities through the period of the data collection. Of the 2698 unique reflections, only 943 exceeded five standard deviations based on counting statistics, indicating the weakness of the diffraction. Absorption was corrected for by Gaussian quadrature integration, and the standard data-reduction corrections were done.

STRUCTURE SOLUTION AND REFINEMENT

Scattering curves for neutral atoms, together with coefficients of anomalous dispersion, were taken from the *International Tables for X-ray Crystallography*, Vol. 4 (Ibers & Hamilton 1974). R and wR indices are of the conventional form and are given as percentages.

The structure was solved by direct methods. The E statistics indicate that the structure is centrosymmetric,

TABLE 3. SELECTED INTERATOMIC DISTANCES (Å) AND ANGLES (°) IN RAPIDCREEKITE

Ca(1)–O(1)	2.350(6)	*Ca*(2)–O(4)	2.472(7)
Ca(1)–O(1)a	2.689(7)	*Ca*(2)–O(5)	2.300(7)
Ca(1)–O(2)	2.366(6)	*Ca*(2)–O(5)b	2.405(7)
Ca(1)–O(2)b	2.499(7)	*Ca*(2)–O(6)c	2.407(6)
Ca(1)–O(3)	2.519(7)	*Ca*(2)–O(6)d	2.538(7)
Ca(1)–O(4)	2.473(7)	*Ca*(2)–O(7)c	2.540(7)
Ca(1)–*W*(1)a	2.461(7)	*Ca*(2)–*W*(3)b	2.440(6)
Ca(1)–*W*(2)b	2.425(6)	*Ca*(2)–*W*(4)	2.504(7)
<*Ca*(1)–O>	2.473	<*Ca*(2)–O>	2.451
S–O(1)	1.457(6)	*C*–O(2)	1.27(1)
S–O(3)b	1.481(7)	*C*–O(4)a	1.31(1)
S–O(6)b	1.475(7)	*C*–O(5)	1.27(1)
S–O(7)	1.461(7)	<*C*–O>	1.28
<*S*–O>	1.469		
Ca(1) polyhedron			
W(1)a–*W*(2)b	3.797(9)	*W*(1)a–*Ca*(1)–*W*(2)b	102.0(2)
Ca(2) polyhedron			
W(3)b–*W*(4)	3.793(9)	*W*(3)b–*Ca*(2)–*W*(4)	100.2(2)
S tetrahedron			
O(1)–O(3)b	2.350(9)	O(1)–*S*–O(3)b	106.3(4)
O(1)–O(6)b	2.421(9)	O(1)–*S*–O(6)b	111.4(4)
O(1)–O(7)	2.419(9)	O(1)–*S*–O(7)	112.4(4)
O(3)b–O(6)b	2.431(9)	O(3)b–*S*–O(6)b	110.7(4)
O(3)b–O(7)	2.401(9)	O(3)b–*S*–O(7)	109.4(4)
O(6)b–O(7)	2.362(9)	O(6)b–*S*–O(7)	107.1(4)
<O–O>	2.397	<O–*S*–O>	109.6
C triangle			
O(2)–O(4)a	2.218(9)	O(2)–*C*–O(4)a	118.4(8)
O(2)–O(5)	2.250(9)	O(2)–*C*–O(5)	124.3(7)
O(4)a–O(5)	2.208(9)	O(4)a–*C*–O(5)	117.2(8)
<O–O>	2.225	<O–*C*–O>	120.0

Symmetry operators: a: $\bar{x}+½, y, z+½$; b: $\bar{x}+½, y, z-½$; c: $\bar{x}+½, y-½, \bar{z}+½$; d: $x, y-½, \bar{z}+1$; e: $\bar{x}, \bar{y}+½, z$; f: $x-½, \bar{y}+½, z+½$; g: $\bar{x}, \bar{y}, \bar{z}+1$; h: $\bar{x}+1, \bar{y}+½, z$; i: $\bar{x}+½, y, z+½$

TABLE 2. FINAL PARAMETERS FOR RAPIDCREEKITE

Site	x	y	z	$^*U_{eq}$	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ca(1)	0.3341(1)	0.2896(1)	0.2009(3)	125(5)	129(9)	106(8)	140(9)	–5(8)	5(12)	1(9)
Ca(2)	0.3276(1)	0.0533(1)	0.1883(3)	127(5)	133(9)	98(9)	149(9)	–2(8)	4(12)	–3(9)
S	0.1688(2)	0.4193(1)	0.0268(4)	127(6)	140(9)	99(9)	143(11)	–21(9)	–13(13)	–20(13)
C	0.1914(5)	0.1739(5)	0.431(1)	113(23)	106(38)	113(39)	120(40)	–12(45)	–24(32)	39(43)
O(1)	0.2247(4)	0.3589(3)	0.050(1)	196(21)	180(35)	158(34)	250(39)	32(33)	–69(34)	80(29)
O(2)	0.2137(4)	0.2329(3)	0.357(1)	150(20)	185(33)	90(31)	175(38)	2(27)	51(29)	–69(28)
O(3)	0.3898(4)	0.4039(3)	0.343(1)	179(20)	162(33)	129(33)	246(39)	–34(30)	40(31)	–27(28)
O(4)	0.3712(3)	0.1714(4)	0.0735(9)	151(17)	165(28)	118(28)	171(31)	–37(35)	–29(27)	8(32)
O(5)	0.2286(4)	0.1168(3)	0.383(1)	170(21)	184(37)	109(31)	216(40)	29(30)	88(29)	7(28)
O(6)	0.2810(4)	0.4830(3)	0.484(1)	166(20)	235(35)	103(31)	160(36)	0(30)	–63(31)	23(29)
O(7)	0.1181(4)	0.4321(3)	0.222(1)	188(21)	203(35)	202(37)	158(36)	1(30)	65(29)	–25(30)
W(1)	0.0894(4)	0.2389(3)	0.013(1)	221(21)	186(34)	231(38)	248(40)	–14(33)	–4(33)	–32(31)
W(2)	0.0478(4)	0.3236(4)	0.466(1)	248(21)	181(30)	307(37)	257(39)	46(41)	–79(30)	–52(38)
W(3)	0.0746(4)	0.0196(3)	0.397(1)	182(20)	173(33)	211(36)	162(35)	18(31)	–60(29)	–53(29)
W(4)	0.4341(4)	0.0914(3)	0.469(1)	200(21)	140(31)	233(40)	226(39)	22(33)	–25(32)	–16(29)

* values quoted are x 10^4.

TABLE 4. BOND-VALENCE* TABLE FOR RAPIDCREEKITE

	Ca(1)	*Ca*(2)	*S*	*C*	H(1)	H(2)	H(3)	H(4)	H(5)	H(6)	H(7)	H(8)	Σ
O(1)	0.33 0.14		1.54										2.01
O(2)	0.31 0.22			1.39		0.1							2.02
O(3)	0.21		1.44							0.2	0.2		2.05
O(4)	0.24	0.24		1.20			0.2						1.88
O(5)		0.37 0.28		1.37									2.02
O(6)		0.28 0.20	1.47										1.95
O(7)		0.20	1.52					0.2					1.92
W(1)	0.25				0.8 0.2	0.8						0.05	2.10
W(2)	0.27						0.8	0.8					1.87
W(3)		0.26							0.8 0.2	0.8		0.05	2.11
W(4)		0.22				0.1					0.8	0.9	2.02
Σ	1.97	2.05	5.97	3.96	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	

* parameters from Brown (1981)

and the solution with the highest combined figure of merit in the space group *Pcnb* gave the structure. Full-matrix least-squares refinement for an anisotropic-displacement model converged to an *R* index of 4.4%. We were unable to definitely locate the H atoms on difference-Fourier maps. However, (OH) and (H_2O) groups were identified on the basis of bond-valence criteria, and are designated as *OH* and *W*, respectively. Final atomic positions and displacement factors are given in Table 2, selected interatomic distances and angles are given in Table 3, and the empirical bond-valence table is shown as Table 4. Observed and calculated structure-factors may be obtained from The Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2.

DISCUSSION

Cation coordination

All sites occupy the general position in rapidcreekite. There is one *C* site coordinated by three oxygen atoms in a triangular arrangement with a <*C*–O> distance of 1.28 Å, a typical value for the (CO_3) group. There is one *S* site coordinated by four oxygen atoms in a tetrahedral arrangement with a <*S*–O> distance of 1.47 Å, in the normal range for the (SO_4) group. There are two distinct *Ca* sites, and their coordinations are very similar (Fig. 1). Each *Ca* is coordinated by six oxygen atoms in the range 2.30–2.69 Å and two (H_2O) groups in the range 2.43–2.50 Å, and a strong pseudosymmetry is apparent between the two coordination polyhedra (Fig. 1).

Topology of the structural unit

The ($Ca\phi_8$) polyhedra (ϕ: unspecified ligand) share edges to form a staggered [$Ca\phi_6$] chain extending along [001] (Fig. 2). One side of the chain links to a (CO_3) group that shares an edge with one ($Ca\phi_8$) polyhedron and a corner with the other ($Ca\phi_8$) polyhedron; the other side of the chain links to an (SO_4) group that also shares an edge with one ($Ca\phi_8$) polyhedron and a corner with the other ($Ca\phi_8$) polyhedron. The resulting

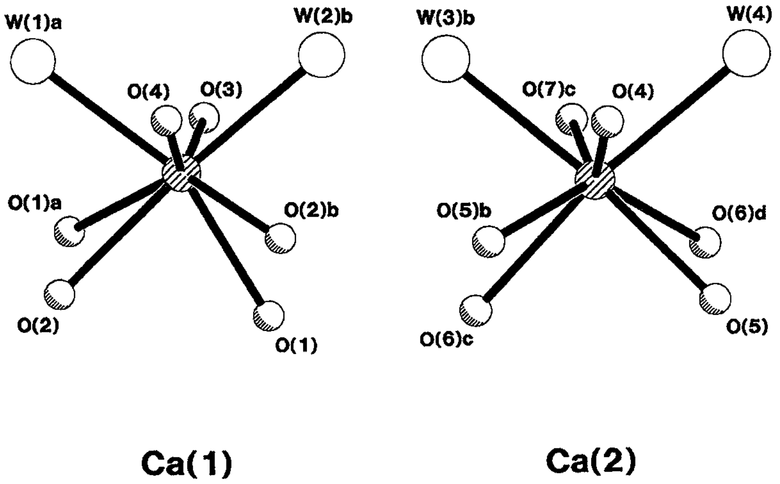


FIG. 1. The Ca(1)ϕ_8 and Ca(2)ϕ_8 coordination polyhedra in rapidcreekite; line-shaded circles: Ca atoms; highlighted circles: O atoms; unshaded circles: H_2O groups.

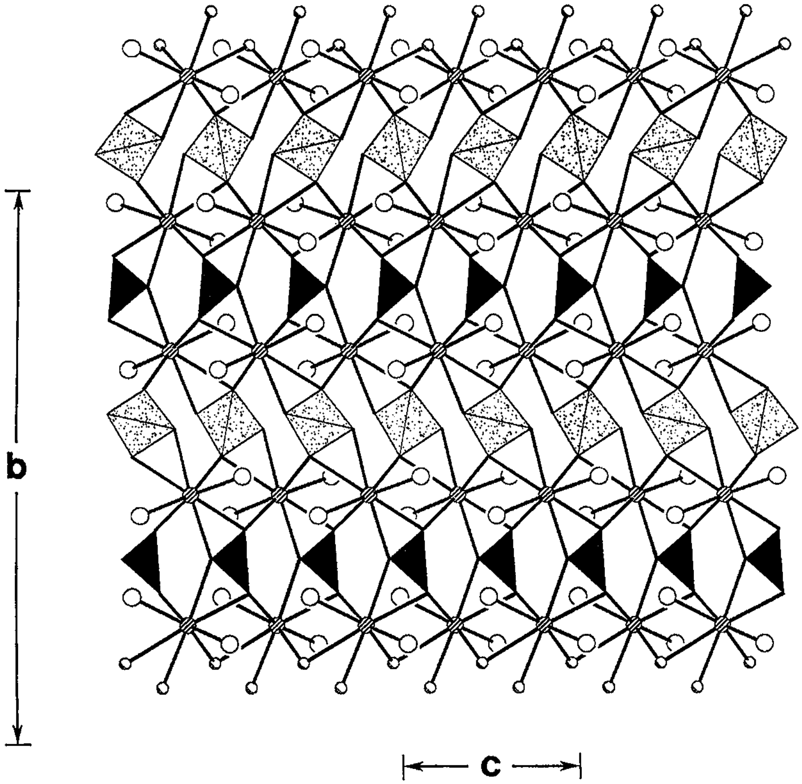


FIG. 2. The structural unit in rapidcreekite, viewed down [100]; the heteropolyhedral sheet consists of chains of edge-sharing $Ca\phi_8$ polyhedra extending along the *c* axis and cross-linked in the *b* direction alternately by strips of CO_3 groups and SO_4 groups. Black triangles: CO_3 groups; random-dot-shaded tetrahedra: SO_4 groups; *Ca* polyhedra and H_2O groups are shown as in Fig. 1.

linkage forms a heteropolyhedral sheet (Fig. 2) that shows extreme compositional layering, chains of $(Ca\phi_8)$ polyhedra alternating with rows of (CO_3) groups and (SO_4) groups. This sheet is parallel to {100} and is the structural unit of rapidcreekite, and has the same chemical composition as the mineral; the structural unit is neutral, and there are no interstitial species.

Hydrogen bonding

We could not locate the H-atom positions directly from the diffraction data. However, a sensible scheme of H-bonding was derived from stereochemical relations and bond-valence arguments. First, all short (*i.e.*, <3.2 Å) *W*–O and *W*–*W* distances were listed. Hydrogen-bond donor–acceptor pairs do not involve anions forming an edge of a single coordination polyhedron (Baur 1972, 1973) (except where the coordination polyhedron involves a monovalent cation of high coordination number), and hence such pairs were deleted from the list of potential donor–acceptor pairs. Next, potential acceptor anions that already had

TABLE 5. PROPOSED H-BONDING FOR RAPIDCREEKITE

ϕ–ϕ	(Å)	H-atom	ϕ–ϕ–ϕ	(°)
* *W*(1)…*W*(1)e	2.808(12)	H(1)	*W*(1)e–*W*(1)–O(2)	132.1(2)
W(1)…O(2)	2.868(9)	H(2)	*W*(1)e–*W*(1)–*W*(4)b	91.5(3)
W(1)…*W*(4)b	2.871(9)	H(2)	O(2)–*W*(1)–*W*(4)b	96.6(3)
* *W*(2)…O(4)f	2.821(8)	H(3)	O(4)f–*W*(2)–O(7)	118.7(3)
W(2)…O(7)	2.793(10)	H(4)		
* *W*(3)…*W*(3)g	2.746(12)	H(5)	*W*(3)g–*W*(3)–O(3)c	101.5(3)
W(3)…O(3)c	2.729(9)	H(6)		
* *W*(4)…O(3)h	2.843(8)	H(7)	O(3)h–*W*(4)–*W*(1)i	96.7(3)
W(4)…*W*(1)i	2.871(9)	H(8)	O(3)h–*W*(4)–*W*(3)i	107.4(3)
W(4)…*W*(3)i	2.978(9)	H(8)	*W*(1)i–*W*(4)–*W*(3)i	111.7(3)

* H-bonding across structural units

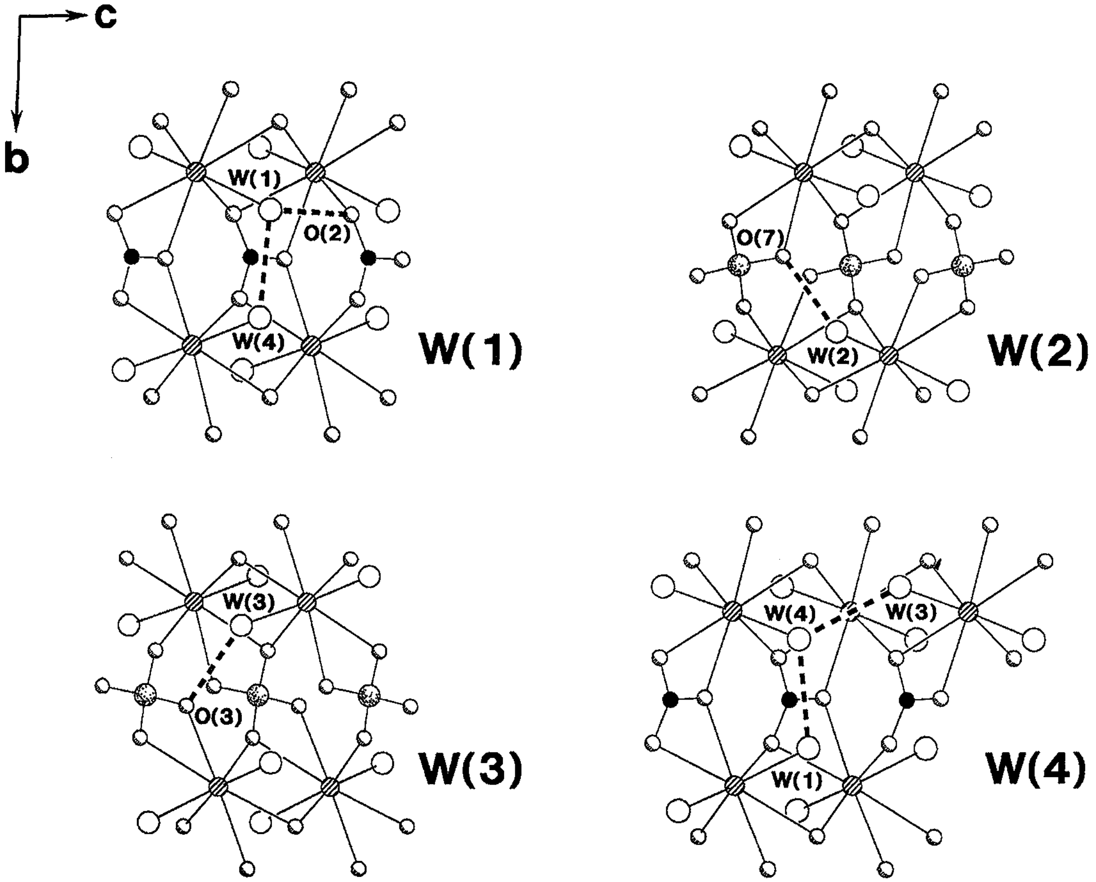


FIG. 3. The *W*-group environments in rapidcreekite viewed down [100]; H-bonds within the plane of the structural unit are shown by heavy broken lines; legend as in Fig. 2.

their bond-valence requirements satisfied by bonds within the structural unit (Table 4) also were removed from the list. The resulting H-bond scheme is shown in Table 5, and the stereochemical details of each (H_2O) group is shown in Figures 3 and 4; Figure 3 shows the H-bonding within the plane of the structural unit, and Figure 4 shows the H-bonding that connects the structural units into a three-dimensional structure. The H(1) atom of the *W*(1) group bonds to a *W*(1) group of the adjacent sheet (Fig. 4, Table 5); the H(2) atom of the *W*(1) group is bifurcated and bonds to both an O(2) atom of the neighboring ($Ca\phi_8$) polyhedron and to a *W*(4) group in the [$Ca\phi_6$] chain across the ribbon of (CO_3) groups (Fig. 3). The H(3) atom of the *W*(2) group bonds to an O(4) atom of an adjacent structural unit (Fig. 4), and the H(4) atom bonds to an O(7) atom of the neighboring (SO_4) group (Fig. 3). The H(5) atom of the *W*(3) group bonds to a *W*(3) group in the adjacent structural unit, and the H(6) atom bonds to an O(3) atom of the neighboring (SO_4) group (Fig. 3). The H(7) atom of the *W*(4) group bonds to an O(3) atom of an adjacent structural unit (Fig. 4) ; the H(8) atom forms a bifurcated H-bond to a *W*(1) group in the next [$Ca\phi_6$] chain and to a *W*(3) group in the same [$Ca\phi_6$] chain.

The inter-unit linkage is shown in Figure 4, where the chemical layering within each structural unit is displayed very prominently. All bonding between structural units involves only weak H-bonds (Tables 4, 5), accounting for the perfect {100} cleavage in rapidcreekite.

Relation to other structures

Rapidcreekite shows strong chemical and structural affinities with gypsum (Atoji & Rundle 1958, Cole & Lancucki 1974, Pedersen & Semmingsen 1982), a mineral with which it occurs. As indicated in Table 6, replacement of half the sulfate groups by carbonate groups in the gypsum formula produces the rapid-

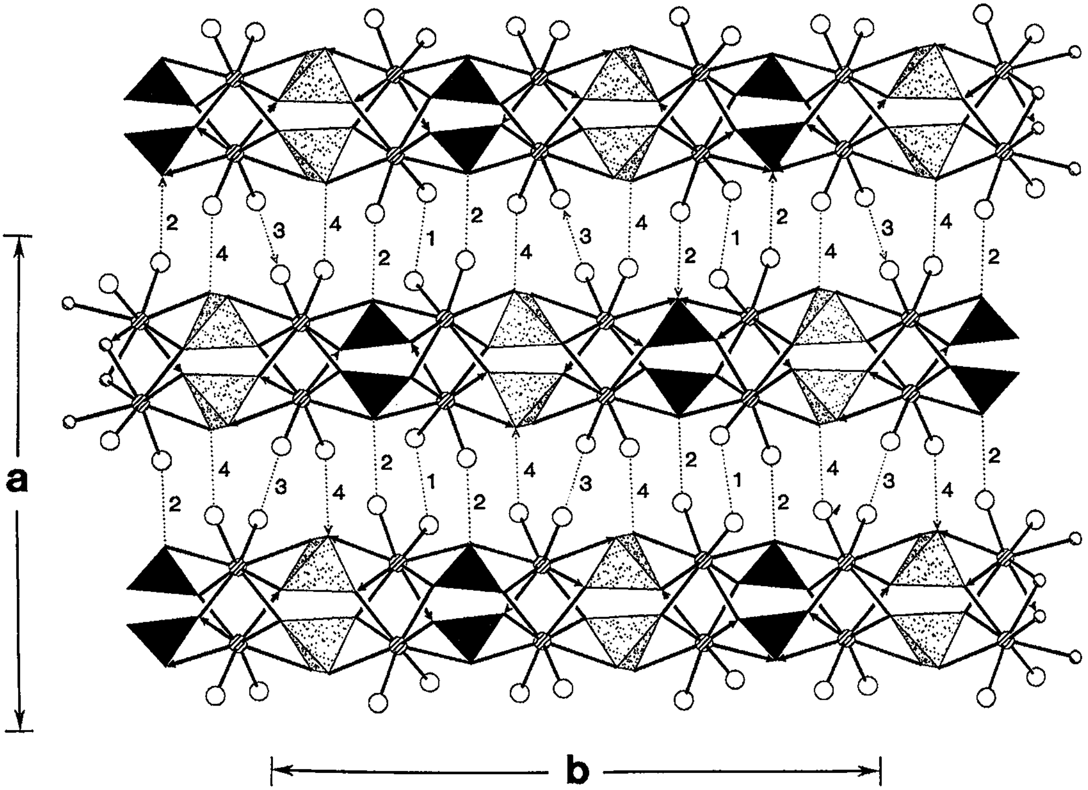


FIG. 4. The structure of rapidcreekite viewed down [001]; legend as in Fig. 2. Adjacent structural units are cross-linked by hydrogen bonding (shown by dotted lines; bonds terminated by arrows link to the corresponding anion one unit-cell length below the plane of the projection. The numbers indicate the following donor–acceptor pairs: 1: *W*(1)...*W*(1); 2: *W*(2)...O(4); 3: *W*(3)...*W*(3); 4: *W*(4)...O(3).

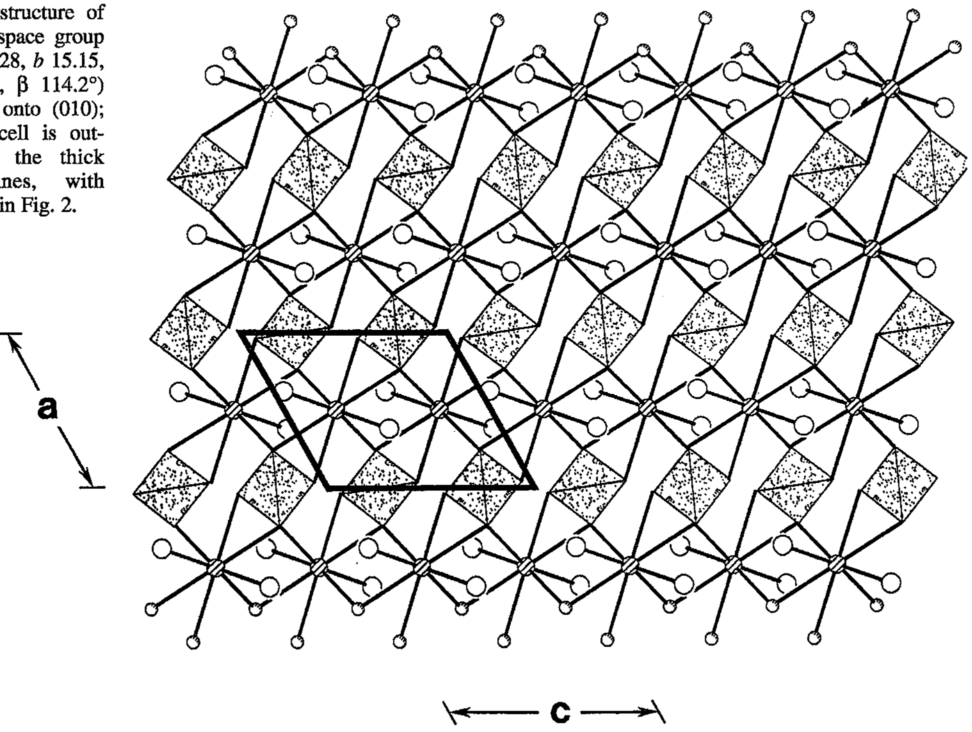
creekite formula. Figure 5 shows a view of the structural unit in gypsum; it is a sheet consisting of chains of edge-sharing Caϕ_8 polyhedra cross-linked into a sheet by rows of (SO_4) groups. The structural unit of gypsum can be transformed into the structural unit of rapidcreekite by twinning along alternate rows of (SO_4) groups. This process is illustrated in Figure 6. At each alternate (SO_4) row, the structure is twinned by rotation of 180° about a [100] axis. This process reverses the cant of the Caϕ_8 polyhedra in adjacent chains (*cf.* Figs. 5, 6) and produces triangles of O atoms at the twin plane (Fig. 6). Occupancy of these triangles by C atoms produces the structural unit in rapidcreekite (Fig. 2).

TABLE 6. CHEMICAL FORMULAE OF GYPSUM, RAPIDCREEKITE AND A HYPOTHETICAL CARBONATE STRUCTURE

Gypsum	Ca_2	(SO_4)	(SO_4)	$4H_2O$
Rapidcreekite	Ca_2	(SO_4)	(CO_3)	$4H_2O$
Hypothetical	Ca_2	(CO_3)	(CO_3)	$4H_2O$

The gypsum structure may twin in this fashion at every row of (SO_4) groups. This would result in a structure consisting of chains of edge-sharing (Caϕ_8) polyhedra linked only by rows of (CO_3) groups (Fig. 7). Although this chemical formula and structural arrangement do not correspond to any known mineral or synthetic compound, there seems no crystal-chemical or structural reason why this arrangement cannot occur. This hypothetical $[Ca_2(CO_3)_2(H_2O)_4]$ sheet somewhat resembles the $[La_2(CO_3)_3(H_2O)_6]$ structural unit of lanthanite (Dal Negro *et al.* 1977). The latter sheet consists of edge-sharing chains of Laϕ_{10} polyhedra cross-linked by (CO_3) groups. Laϕ_{10} polyhedra are canted in different directions in adjacent chains, and alternate rows of (CO_3) groups point in

FIG. 5. The structure of gypsum (space group *C2/c*, *a* 6.28, *b* 15.15, *c* 5.67 Å, β 114.2°) projected onto (010); the unit cell is outlined by the thick black lines, with legend as in Fig. 2.



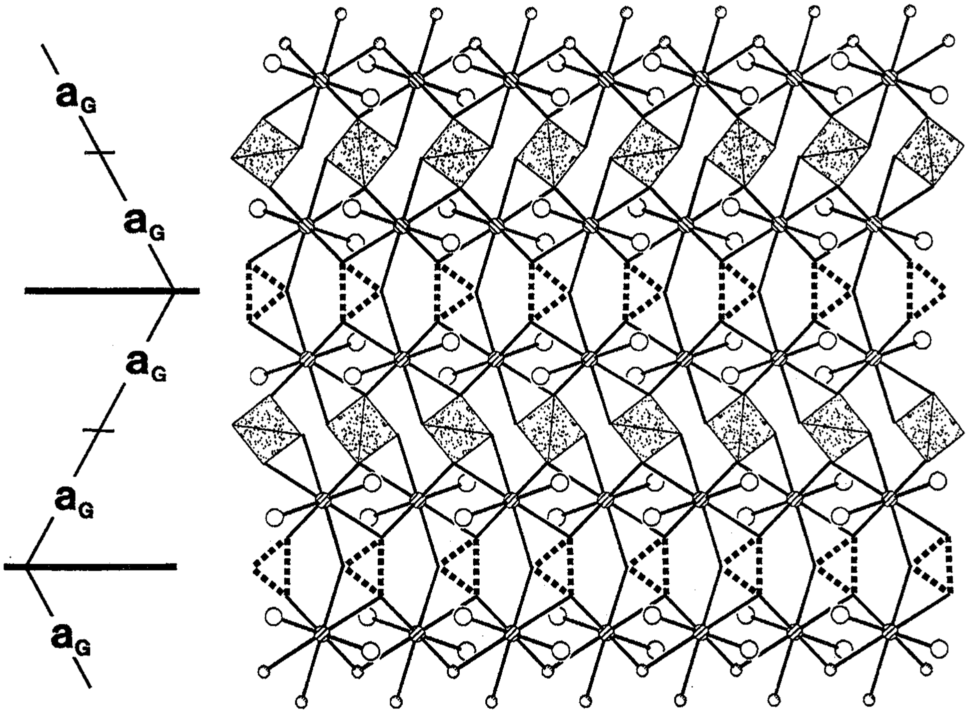


FIG. 6. The building mechanism of rapidcreekite from the gypsum structure. At each alternate row of (SO_4) groups in the gypsum structure (marked by thick black lines to the left of the structure), the structure is twinned by a two-fold rotation about the [100] axis. This operation reverses the tilt of alternate rows of $(Ca\phi_8)$ polyhedra and forms triangles of O atoms (shown in heavy broken lines) at each twin boundary.

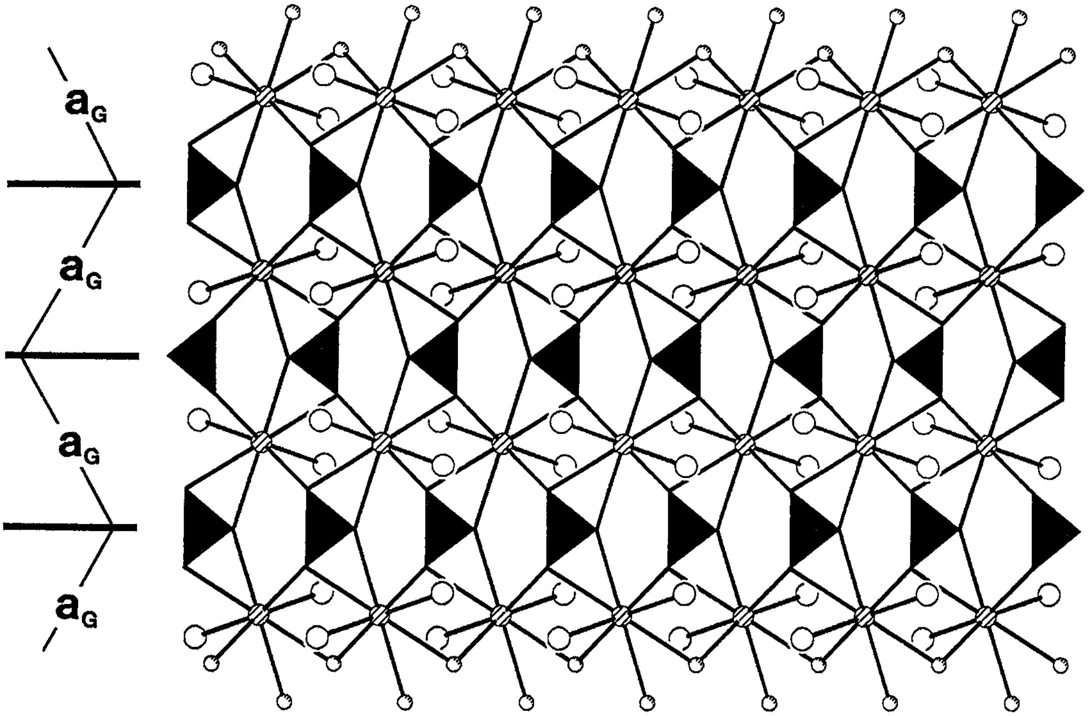


FIG. 7. A hypothetical carbonate structure of composition $CaCO_3(H_2O)_2$ formed by twinning the gypsum structure (Fig. 5) every (SO_4) row (thick lines at the left of the figure).

opposite directions. However, the sheet in lanthanite differs by having an additional (CO_3) group per La cation decorating the surface of the sheet; each (CO_3) group provides an additional two ligands per La cation necessary for La to achieve [10]-coordination.

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