

Figure 1. a) Unit cell of $\text{Na}_2[\text{FeS}_6]$. b) Unit cell of $\text{Na}_4[\text{Fe}_2\text{S}_6]$. c) Acentric dimer1 (left) and centrosymmetric dimer2 (right) with Na^+ coordination. Bridging and terminal Fe-S bond lengths of dimer1 / dimer2: $d_{\text{Fe-S}}^{\text{br}} = 234.7(3) / 235.4$ pm, $d_{\text{Fe-S}}^{\text{t}} = 228.7(1) / 229.2(2)$ pm.

Keywords: chalcogenido ferrate, diferrate, band structure, magnetism

MS15-P22 The biclinic crystal system – a hidden system in crystallography

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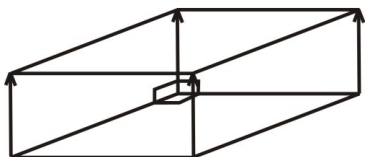
It is well known that there are seven crystal systems, the cubic, hexagonal, trigonal, tetragonal, orthorhombic, monoclinic and the triclinic systems. From the orthorhombic to the triclinic systems, the crystal axial angles change from orthogonal ($\alpha = \beta = \gamma = 90^\circ$) to oblique in one axis (e.g. $\beta \neq 90^\circ$) to oblique in three axes ($\alpha \neq \beta \neq \gamma \neq 90^\circ$). There is no oblique case in two axes (any two of α , β and $\gamma \neq 90^\circ$ and with the remainder = 90°). That is strange. The biclinic crystal system ($a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$ and α (or β or γ) = 90°) is a real but being hidden system in crystallography. As α (or γ) = 90° ($\beta \neq \gamma \neq 90^\circ$ or $\beta \neq \alpha \neq 90^\circ$), kaolinite donates a real example of the biclinic crystal system [1]. The formation of the biclinic system is demonstrated by its equivalent biclinic-parallelepiped that is built from a pair of rectangles by shifting each other along their two edges (Fig. 1). The P1 and P-1 properties of space group are deduced from both twofold axis and mirror plane. Those formulae of the biclinic system are given for useful calculations including the metric tensor G and its reciprocal G-1, volume V, reciprocal lattice parameters a^* , b^* , c^* , α^* , β^* and γ^* , the relationships between the Miller indices, interplanar angle Φ , vector length r , intervector angle ρ and the interplanar distance d . The transformations between the biclinic and the triclinic crystal systems arisen from a little axis-angle variations are exemplified with kaolinite, heulandite and anorthite. It is summarized from those transformations that the difference, in d spacing, less than 0.05° 2θ in copper radiation will be no significance in distinguishing the biclinic from the triclinic system and *vice versa* [2]. It is worth noting that when use the regulations of the triclinic system to deal with these data of the biclinic system it is very easy to fall in a “no biclinic system” trap and layouts them into the triclinic system. Finally, the “missing” of the biclinic crystal system is because the P1 and P-1 space groups are classified into the triclinic system. One does not need to “refine” the data ($a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$ and α or β or $\gamma = 90^\circ$) from the biclinic system to the triclinic system ($\alpha \neq \beta \neq \gamma \neq 90^\circ$). These low grade crystal systems (bi- and triclinic) would make a plentiful crystal world.

References

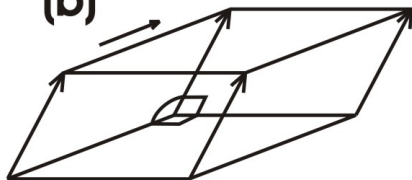
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(a)



(b)



(c)

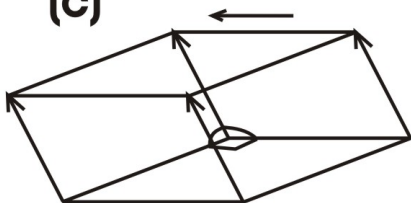


Figure 1. Formation of the biclinic parallelepiped. (a): orthorhombic parallelepiped, (b): monoclinic parallelepiped, (c): biclinic parallelepiped.

Keywords: crystal system, space group, formulae, kaolinite

MS15-P23 Crystal Structure of a New Coordination Polymer

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The oxalate dianion is one of the most studied ligands, capable of bridging two or more metal centres and creating inorganic polymers based on the assembly of metal polyhedra with a wide variety of one-, two - or three dimensional extended structures. Among the oxalate-based compounds M with the general formula $AM(C_2O_4)_n(H_2O)$ (A= alkali metal and, M= trivalent element), only a few crystal structures involving sodium metal have been reported in the literature with $M=Yb$ [1]. As a continuation of work on mixed oxalate-based compounds with a tri- or bivalent element [2] a new coordination polymer, namely catena-poly[[diaquasodium(I)]- μ -oxalato- $k^4O1,O2:O1',O2'$ -[diaquairon(III)]- μ -oxalato- $k^4O1,O2:O1',O2'$], $[NaFe(C_2O_4)_2(H_2O)_4]_n$, has been prepared and its crystal structure elucidated by single-crystal X-Ray diffraction analysis [3]. The compound crystallizes in the non centrosymmetrical space group $I4_1$ ($Z = 4$). The asymmetric unit contains one Na(I) atom and one Fe(III) atom lying on a fourfold symmetry axis, one oxalate ligand and two aqua ligands. Each metal atom is surrounded by two chelating oxalate ligands and two equivalent water molecules, in a *cis* arrangement. The structure consists of infinite one-dimensional chains of alternating $FeO(H_2OW)_2$ and $NaO(H_2OW)_2$ octahedra, bridged by oxalate ligands, parallel to the $[100]$ and $[010]$ directions, respectively (Fig. 1). Because of the *cis* configuration and the μ_2 -coordination mode of the oxalate ligands, the chains run in a zigzag manner. This arrangement facilitates the formation of hydrogen bonds between neighboring chains involving the H_2O and oxalate ligands, leading to a two-dimensional framework. The resulting framework exhibits tunnels parallel to the *c* axis with an elliptic cross-section as shown in Fig. 1. The structure of this new one dimensional coordination polymer is shown to be unique among the $A^I M^{III}(C_2O_4)_2(H_2O)_n$ series. The thermal decomposition behavior has been studied by TG and DTA and gave as a final product the well-known ternary oxide $NaFeO_2$ [1] Chapelet-Arab B., Duvieubourg, L., Nowogrocki G., Abraham F., Grandjean S. (2006). *J. Solid State Chem.* **179**, 4029 [2] Kherfi H., Hamadène M., Guehria A., Dahaoui S. & Lecomte C. (2011). *Acta Cryst.* **C67**, m85 (2013). *Acta Cryst.* **E69**, m493 [3] Benhacine M.A., Hamadène M., Bouacida S., Mérazig H. (2016). *Acta Cryst.* **C72**, 243

Keywords: absolute structure, one-dimensional chains, new structural type