

## 9.2. LAYER STACKING

Weiss & Đurovič, 1983). The papers published before 1983 use the Pauling model; the later papers are based on the model of Radoslovich (1961) with *trigonal* symmetry of tetrahedral sheets. In all cases, MDO polytypes (§9.2.2.2.3) have been derived systematically: their sets partially overlap with basic polytypes presented by the US or the USSR schools. The OD models allowed the use of unitary descriptive symbols for individual polytypes from which all the relevant symmetries can be determined (Đurovič & Dornberger-Schiff, 1981) as well as of extended indicative Ramsdell symbols (Weiss & Đurovič, 1985b). The results, including principles for identification of polytypes, have been summarized by Đurovič (1981).

The main features of polytypes of basic types of hydrous phyllosilicates, of their diffraction patterns and principles for their identification, are given in the following.

## 9.2.2.3.1.1. General geometry

Tetrahedral and octahedral sheets are the fundamental, *two-dimensionally periodic* structural units, common to all hydrous phyllosilicates. Any *tetrahedral sheet* consists of  $(\text{Si,Al,Fe}^{3+},\text{Ti}^{4+})\text{O}_4$  tetrahedra joined by their three basal O atoms to form a network with symmetry  $P(3)1m$  (Fig. 9.2.2.6a). The atomic coordinates can be related either to a hexagonal axial system with a primitive unit mesh and basis vectors  $\mathbf{a}_1, \mathbf{a}_2$ , or to an orthohexagonal system with a *c*-centred unit mesh and basis vectors  $\mathbf{a}, \mathbf{b}$  ( $b = \sqrt{3}a$ ). Any *octahedral sheet* consists of  $M(\text{O,OH})_6$  octahedra with shared edges (Fig. 9.2.2.6b), and with cations *M* most frequently  $\text{Mg}^{2+}, \text{Al}^{3+}, \text{Fe}^{2+}, \text{Fe}^{3+}$ , but also  $\text{Li}^+, \text{Mn}^{2+}$  ( $r_M < \sim 0.9 \text{ \AA}$ ), etc. There are three octahedral

sites per unit mesh  $\mathbf{a}_1, \mathbf{a}_2$ . Crystallochemical classification distinguishes between two extreme cases: *trioctahedral* (all three octahedral sites are occupied) and *dioctahedral* (one site is – even statistically – empty). This classification is based on a bulk chemical composition. A classification from the symmetry point of view distinguishes between three cases: *homo-octahedral* [all three octahedral sites are occupied by the same kind of crystallochemical entity, *i.e.* either by the same kind of ion or by a statistical average of different kinds of ions including voids; symmetry of such a sheet is  $H(3)12/m$ ];\* *meso-octahedral* [two octahedral sites are occupied by the same kind of crystallochemical entity, the third by a different one, in an ordered way; symmetry  $P(3)12/m$ ]; and *hetero-octahedral* [each octahedral site is occupied by a different crystallochemical entity in an ordered way; symmetry  $P(3)12$ ]. The prefixes homo-, meso-, hetero- can be combined with the prefixes tri-, di-, or used alone (Đurovič, 1994).

A tetrahedral sheet (*Tet*) can be combined with an octahedral sheet (*Oc*) either by a shared plane of apical O atoms (in all groups of hydrous phyllosilicates, Fig. 9.2.2.7a), or by hydrogen bonds (in the serpentine-kaolin group and in the chlorite group, Fig. 9.2.2.7b). Two tetrahedral sheets can either form a pair anchored by interlayer cations (in the mica group, Fig. 9.2.2.8a) or an unanchored pair (in the talc-pyrophyllite group, Fig. 9.2.2.8b).

The ambiguity in the stacking occurs at the centres between adjacent *Tet* and *Oc* and between adjacent *Tet* in the talc-pyrophyllite group. From the solved and refined crystal structures it follows that the displacement of (the origin of) one sheet relative to (the origin of) the adjacent one can only be one (or simultaneously three – for homo-octahedral sheets) of the nine vectors shown in Fig. 9.2.2.9.

The number of possible positions of one sheet relative to the adjacent one can be determined by the corresponding NFZ relations (§9.2.2.2.1). As an example, the contact (*Tet*; *Oc*) by shared apical O atoms, and the contacts (*Oc*; *Tet*) by hydrogen

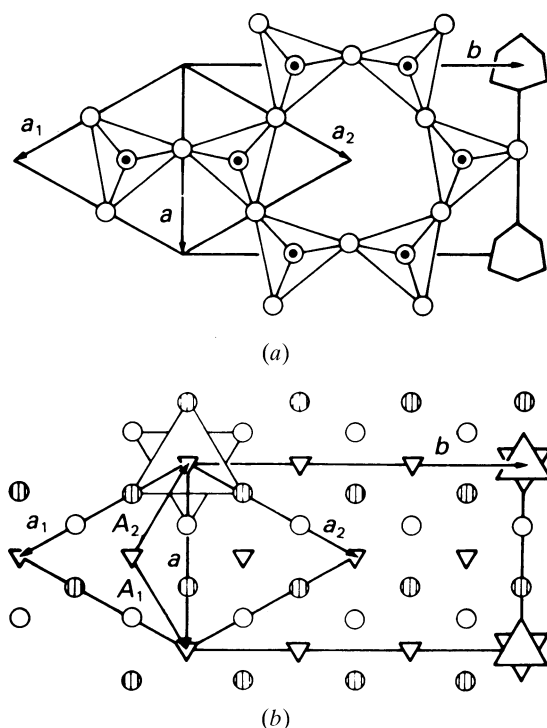


Fig. 9.2.2.6. (a) Tetrahedral sheet in a normal projection. Open circles: basal oxygen atoms, circles with black dots: apical oxygen atoms and tetrahedral cations. Hexagonal and orthohexagonal basis vectors and symbolic figures (ditrigons) for pictorial representation of these sheets are also shown. (b) Octahedral sheet. Open and shaded circles belong to the lower and the upper oxygen atomic planes, respectively; small triangles denote octahedral sites. Triangular stars on the right are the symbolic figures for pictorial representation of these sheets: the two triangles correspond to the lower and upper basis of any octahedron, respectively.

\* A hexagonally centred unit mesh  $\mathbf{a}_1, \mathbf{a}_2$  instead of a primitive mesh  $\mathbf{A}_1, \mathbf{A}_2$  is used (Fig. 9.2.2.6b).

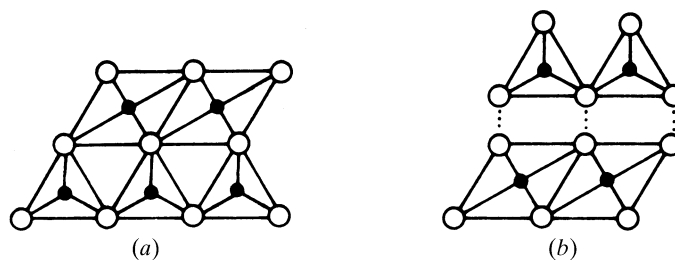


Fig. 9.2.2.7. Two possible combinations of one tetrahedral and one octahedral sheet (a) by shared apical O atoms, (b) by hydrogen bonds (side projection).

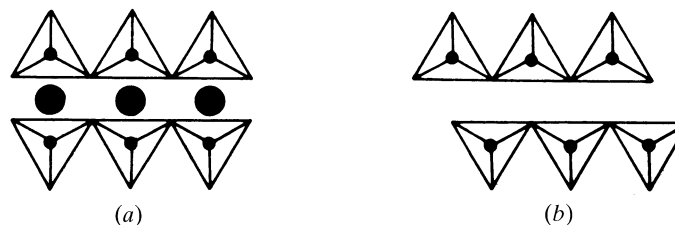


Fig. 9.2.2.8. Combination of two adjacent tetrahedral sheets (a) in the mica group, (b) in the talc-pyrophyllite group (side projection).