

Appendix

This appendix provides the definition of selected structural parameters mentioned in the body of the text.

Tetrahedral Rotation angle, α .

Tetrahedral rotation angle (α) was defined according to the following formula:

$$\alpha = \frac{\sum_i^6 |120 - \varphi_i|}{12} \quad (1)$$

Where φ_i is a generic internal angle of the hexagon defined by basal O atoms.

Variance of A-O_{basal} distances, σ A-O_{basal}

This parameter is a measure of the distortion of interlayer coordination and can be computed from:

$$\sigma A - O_{\text{basal}} = \sqrt{\frac{\sum_i (A - O_{\text{basal},i} - \langle A - O_{\text{basal}} \rangle)^2}{n}} \quad (2)$$

where A-O_{basal,i} is an individual interlayer cation (A)-basal O atom distance; (O_{basal,i})(A-O_{basal}) is the mean interlayer cation-basal O distance; n is the number of individual interlayer cation-basal O atom distances (e.g., 12).

Mean interlayer cation (A)–tetrahedral cation (T) distances, projected on (001) plane, (A-T)₍₀₀₁₎.

This parameter is the average of individual (A-TO_i)₍₀₀₁₎ components, where T_i is a generic tetrahedral cation and the following relationships apply:

$$(A-TO_i)_{(001)} = (A-TO_i)_{\text{h}} \quad (3)$$

$$\text{h} = \text{i} \times \text{j} \quad (4)$$

$$(A-T_i)_{(001)} = \sqrt{(A-T_i)^2 - (A-T_i)_{(001)}^2} \quad (5)$$

Variance of (A-T)₍₀₀₁₎, σ (A-T)₍₀₀₁₎

See the definition of σ A-O_{basal}, for the definition of variance, and of (A-T)₍₀₀₁₎.

Distance between interlayer cation (A) and individual tetrahedral cation T1_{M1}, as defined in Figure 1, projected on (001), A-T1_{M1, (001)}

See the definition of (A-T)₍₀₀₁₎.

Distance between interlayer cation (A) and anionic position (O4), projected on (001), A-O4₍₀₀₁₎

See the definition of (A-T)₍₀₀₁₎.

Distance between interlayer cation (A) and octahedral cation M1, projected on (001), A-M1₍₀₀₁₎

See the definition of (A-T)₍₀₀₁₎.