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, σA-O_{basal}

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

$$\acute{o}A - O_{basal} = \sqrt{\frac{\Sigma_i \left(A - O_{basal,i} - \langle A - O_{basal} \rangle\right)^2}{n}} \quad (2)$$

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:

$$(A–TO_i)_{[001]} = (A–TO_i)\text{~~n~~} \quad (3)$$

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

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

Variance of (A-T)$_{(001)}$, σ(A-T)$_{(001)}$

See the definition of σA-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)$_{(001)}$.