

Supplementary material

Figure 1

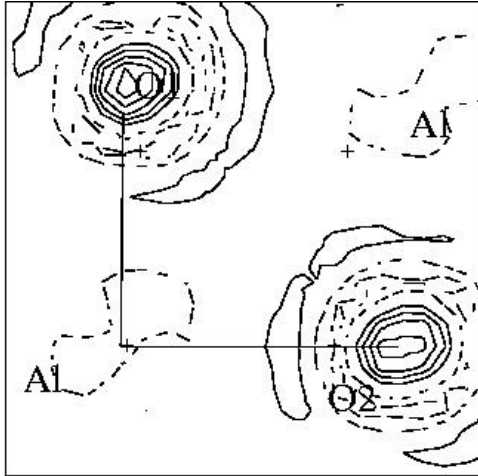
Residual density in the O₁-Al-O₂ plane, all data are after κ_{L-Al} core refinement for Al: (a) WD data ; (b) WDN data ; (c) CD data. Contours are plotted at 0.01 e Å⁻³, negative contours dashed, zero contour omitted.

Figure 2

Static deformation density in the O₁-Al-O₂ plane passing through 2 Al and 2 O atoms and showing the 2 different Al-O bonds: (a) obtained from MOLLY refinement ($\square_{max}=4$) with WSN data ; (b) obtained from MOLLY refinement ($\square_{max}=4$) with CD data. Contours are plotted at 0.05 e Å⁻³ intervals, zero contour dotted, negative dashed.

Figure 3

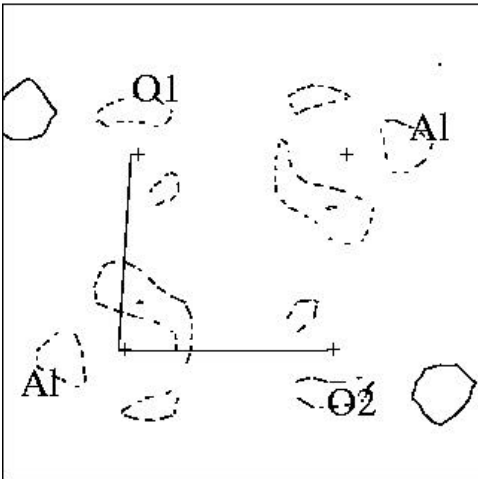
Static deformation density in the O₂-O₃-O₄ plane perpendicular to the c axis, passing only through oxygen atoms. Point C is the center of the common face between two Al octahedra: (a) obtained from MOLLY refinement ($\square_{max}=4$) with WS data ; (b) obtained from MOLLY refinement ($\square_{max}=4$) with WD data ; (c) obtained from MOLLY refinement ($\square_{max}=4$) with WDN data ; (d) obtained from MOLLY refinement ($\square_{max}=4$) with CD data ; (e) obtained from MOLLY refinement ($\square_{max}=4$) with LSF data ; (f) obtained from MOLLY refinement ($\square_{max}=4$) with GS data. Contours as Figure 2.



(a) WD

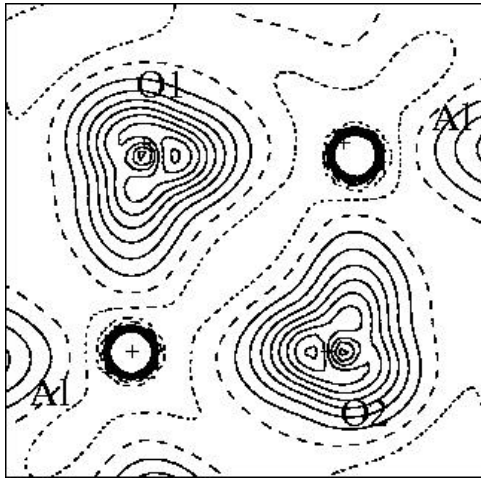


(b) WDN

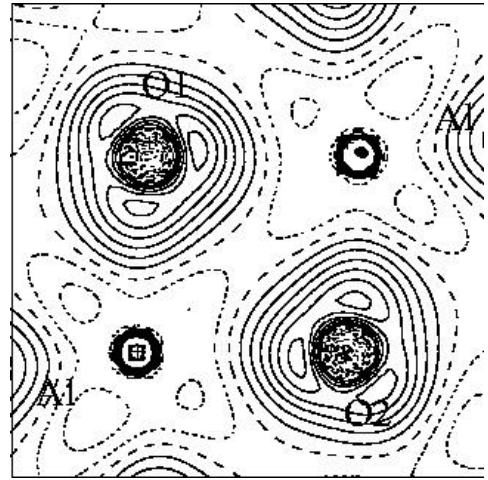


(c) CD

Figure 1

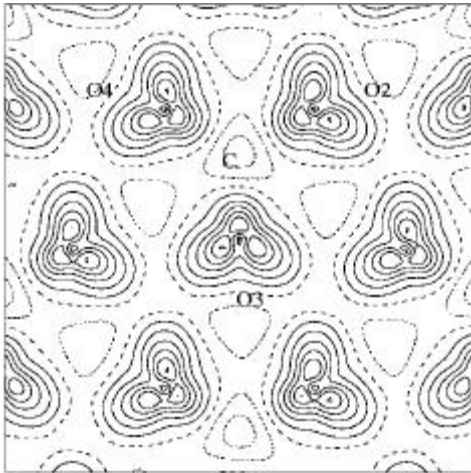


(a) WSN

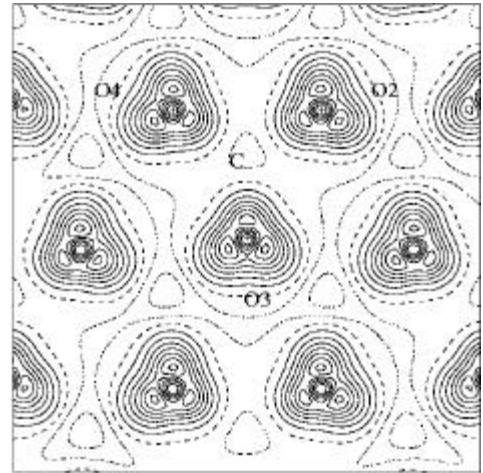


(b) CD

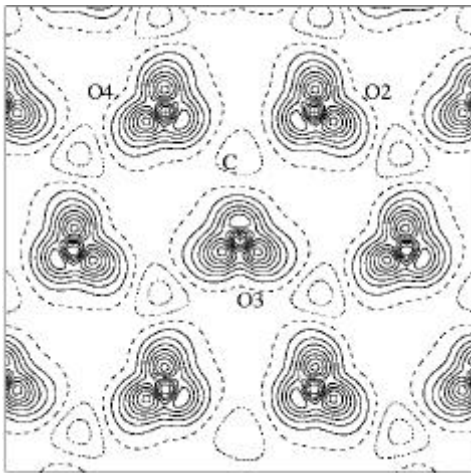
Figure 2



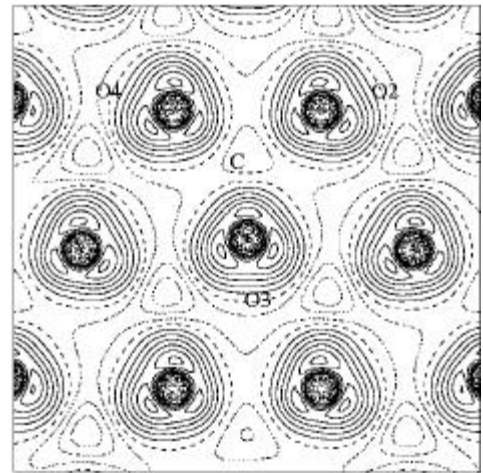
(a) WS



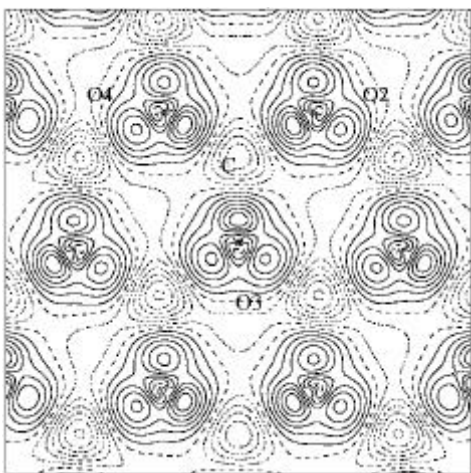
(b) WD



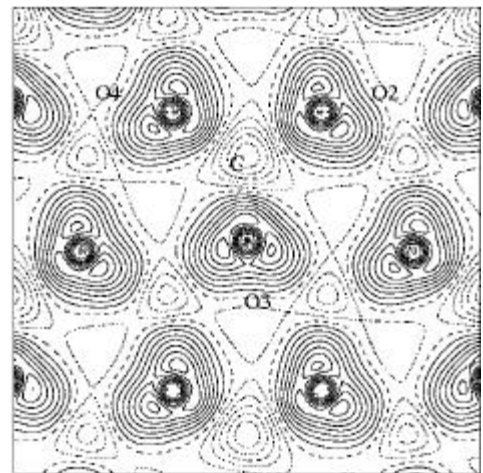
(c) WDN



(d) CD



(e) LSF



(f) GS

Figure 3