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Electric field gradient tensors at the aluminum sites in the Al_2SiO_5 polymorphs from CCD high-resolution X-ray diffraction data: Comparison with ^{27}Al NMR results

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ABSTRACT

High-resolution single-crystal X-ray diffraction intensities recorded with a charge-coupled device detector at low temperature (100 K) were used to derive the electron density distribution in three Al_2SiO_5 polymorphs: andalusite, sillimanite, and kyanite. The ^{27}Al nuclear quadrupole coupling tensors were estimated from both the internal polarization contribution of the Al electron density and that of the lattice with electronic multipoles up to octupoles for oxygen atoms and hexadecapoles for Si and Al. Based on new estimations of the ^{27}Al Sternheimer shielding factor, R and the antishielding factor, γ, a close agreement was achieved between the quadrupole coupling tensors at the various Al-sites derived from the X-ray diffraction data for all three polymorphs of Al_2SiO_5 with those determined previously from single-crystal ^{27}Al NMR spectra.