The residual electron density distribution in spinels
H. Sawada Col. Humanities and Sci., Nihon Univ.

A recent single crystal X-ray diffraction study (H. Sawada, Mat. Res. Bull. 30-3, 341) on MgAl_{2}O_{4} spinel has shown a residual electron density peak with
>0.7 \, \text{e/Å}^{3} \text{ height in the center of the } \text{Al}_{4}\text{O}_{4} \text{ cuboid in the structure, persisting through all modes of refinement, from isotropic (/ harmonic) to anharmonic, with or without application of a novel procedure employed to obtain experimental scattering factors. With no evidence of coexistence of an alternate motif (e.g. inverted } \text{MgO}_{4} \text{ tetrahedra-}\text{AlO}_{4} \text{ cuboids' sequence, local substitution of tetrahedra for cuboids, etc.) the cuboid center seems to be a site which may reflect the chemical or physical characteristics of compounds assuming this structure.}

Results on crystal structure refinements performed on several compounds with spinel structure are to be reported.

Difference Fourier section of a plane \( x=y \) for MgAl_{2}O_{4} (scattering factor refined, anharmonic). Position C denotes the position of the cuboid center. Map borders 5×3Å, increment of contours 0.05\, \text{e/Å}^{3}, negative contours dotted, zero dashed.