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STRUCTURAL STUDIES OF GRAPHITE INTERCALATION COMPOUNDS OF ANTIMONY CHLORIDEFLUORIDES USING (001) X-RAY REFLEXIONS

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X-ray diffraction studies were made for $SbCl_5$, $SbCl_4F$, $SbCl_2F_3$ and SbF_5 graphite intercalation compounds of stages 1, 2 and 3. The (001) reflex intensities were analyzed in terms of a centrosymmetric structural model showing periodic layer stacking, with chlorine layers contacting antimony as well as carbon layers. The results are in agreement with the structural model recently found in other metal halide graphites. Contrary to the classical model, a displacement (about 0.35 Å) of the Sb atoms from the mirror plane in the centre of the intercalant layer was found. Thus in projection onto the c-axis different distances between antimony and halogen atoms result. The analyses of different stages of one compound lead to similar layer parameters. The positions of the five halogen atoms in each compound were refined using a unique z-coordinate. However, it seems reasonable that the halogen atoms are arranged in different z-coordinates.

In case of dilute $SbCl_5$ graphites prepared in CCl_4 solution, the identity period along c-axis I_c increases with $SbCl_5$ concentration in the stage 2 compound. X-ray analysis reveals that Sb atoms move towards the mirror plane, when the $SbCl_5$ concentration increases. In agreement to Moessbauer studies it has to be assumed that the gallery is filled by SbX_5 trigonal bipyramids, and the molecular axis is tilted with respect to the c-axis. The shifting of molecules towards the centre may be due to the fact that polymeres linked by halogen bridges are formed.