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APPLICATION OF ESCA, EXAFS AND NMR SPECTROSCOPY TO THE STUDY OF GRAPHITE INTERCALATION COMPOUNDS WITH HALOGEN FLUORIDES

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By means of ESCA, IR, and NMR - F^{19} spectroscopy in graphite intercalation compounds (GIC) containing ClF_3(1), ClF_5(2), BrF_3(3), and BrF_5(4) two types of C - F bonds are identified.More intensive components in spectra are characteristic for (C - F) bonds of GIC with halogen fluorides and the less intensive ones represent $(CF)_x$ groops.The corresponding parameters of abovementioned spectra for (C - F) bonds are: C 1s - 288.5 eV, F 1s - 689.4 eV; IR peak position - 1130 cm^{-1}, NMR chemical shift - 564 ppm.A possible origin of two additional ESCA peaks of C 1s positioned at 286.8 eV (intensive) and 291.6 (weak) is discussed breifly.

An analysis of the EXAFS data for (3) and (4) compounds shows that corresponding interatomic distances Br-Br, Br - F and Br - C are close to that known in literature for Br_2, BrF_3 and organic compounds (CBr_4).

An analysis of the amplitudes and of the peak positions of the Fourier transformed EXAFS spectra made it possible to evaluate the spatial distribution of BrF_3 molecules in GIC crystal lattice.Dimers $(BrF_3)_2$ and polymers $(BrF_3)_n$ may be revealed by such an analysis.