THE VAPOUR PHASE COMPLEX $AlF_3 \cdot 2HF$ AN AB-INITIO MOLECULAR ORBITAL STUDY

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The complex $AlF_3 \cdot HF$ has been detected by mass spectrometry during the evaporation of pure AlF_3, $Al(OH)F_2 \cdot H_2O$ and $(H_3O)_3AlF_6 \cdot 3H_2O$ in the temperature range between 300 and 400 °C. The complex $AlF_3 \cdot 2$ HF has been observed above 850 °C if the partial pressure of HF was sufficient in the beginning of the AlF_3 evaporation. Available experimental methods for the structure determination are presently not applicable. In order to gain information about the structure and the bonding situation of the complex, Hartree-Fock calculations using extended basis sets like DZP and TZ2P have been performed. A cyclic minimum energy structure, built of weakly distorted HF and AlF_3 molecules has been found. Therefore the complex can be described as an electron pair donor acceptor adduct. Corrections for the basis set superposition error (BSSE) and thermodynamics were proven to be absolutely necessary. The BSSE using the very extended TZ2P basis for example is still in the order of 10 % of the calculated bonding energy.