INFRARED SPECTRA OF $SF_6^- \cdot (H_2O)_n$ ($n = 1 - 3$): INCIPIENT REACTION AND DELAYED ONSET OF WATER NETWORK FORMATION

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We present data on the microhydration environment of the SF_6^- anion, which can serve as a prototype species to investigate the interaction of an extended negative charge distribution with water ligands. This is particularly interesting, given that there are few data on such large systems, while the hydration of small anions such as halides is already well understood. Our infrared spectra of the $SF_6^- \cdot (H_2O)_n$ ($n = 1 - 3$) clusters suggest that the first two water molecules attach to the SF_6^- anion via single ionic H bonds to the same F atom, while signatures of H-bonded networks occur only in the spectrum of the trihydrate. This is an unusual observation as water-water H bonding usually sets in already at the dihydrate level. In addition, we find the SF bond involved in hydrogen bonding considerably weakened upon attachment of the first two ligands, hinting at a possible mechanism for reactions of pre-formed hydrated SF_6^- anions in collisions with water molecules observed in flow-tube experiments.