

Infrared Spectrum of Hydrogen Fluoride Anion Isolated in Solid Argon

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Hypervalent molecules are one of the exceptions to the octet rule. Bonding in most hypervalent molecules is well rationalized by the Rundle-Pimentel model (three-center four-electron bond), and high ionic bonding between the ligands and the central atom is essential for stabilizing hypervalent molecules. Here, we produced one of the simplest hypervalent anions, HF^- , which is known to deviate from the Rundle-Pimentel model, and identified its ro-vibrational features shown in Fig. 1. High-level ab initio calculations reveal that its bond dissociation energy is comparable to that of dihalides, as supported by secondary photolysis experiments with irradiation at various wavelengths. The charge distribution analysis suggested that the F atom of HF^- is negative and hypervalent and the bonding is more covalent than ionic.

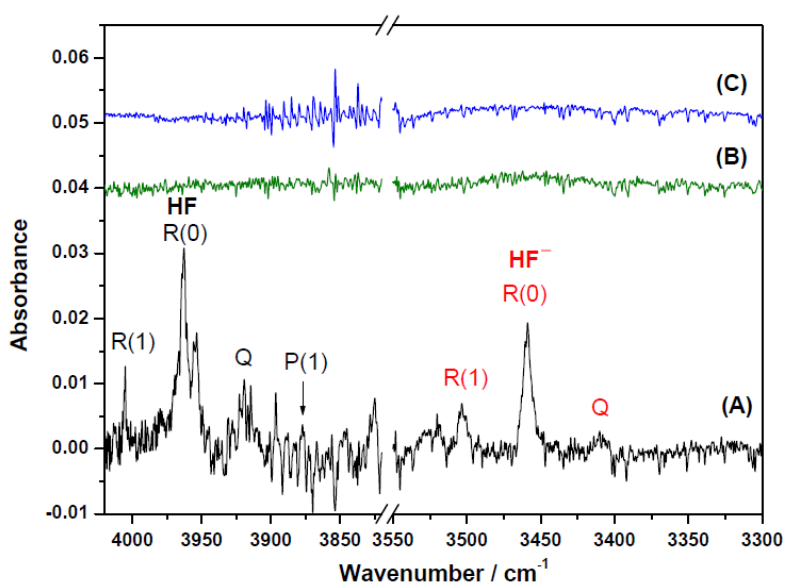


Fig. 1 Partial IR spectra of electron-bombarded (2000 eV, 0.3 mA) matrix samples at 10 K. (A) $\text{CH}_3\text{F}/\text{Ar}$ (1/500), (B) CH_4/Ar (1/500), and (C) Ar. The ro-vibrational transitions of the observed bands are assigned.