

## Matrix isolation study of difluoromethane radiolysis: formation of unusual intermediates and novel noble gas compounds

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Difluoromethane is widely used as an ecologically friendly alternative to conventional chlorofluorocarbons (CFCs). Being chemically and photochemically inert and insensitive to the near UV light, CH<sub>2</sub>F<sub>2</sub> could come to the upper layers of the atmosphere, where it is subjected to VUV or ionizing radiation. The combined matrix isolation and quantum chemistry investigation of difluoromethane radiation-induced transformations is of particular interest for atmospheric chemistry. On the other hand, these studies may provide unique information on the structure and spectroscopic features of intermediates and noble gas compounds.

In this work, we report a FTIR matrix isolation study on the radiolysis and post-irradiation thermal reactions occurring in CH<sub>2</sub>F<sub>2</sub>/Ng and CH<sub>2</sub>F<sub>2</sub>/N<sub>2</sub>O/Ar systems (Ng = Ar, Kr, Xe). The deposited samples were irradiated with X-rays (45 kVp) at 6 K. The assignment of spectral features was based on the ab initio calculations at the CCSD(T)/Lx\_3 levels of theory.

The principal radiolysis products of CH<sub>2</sub>F<sub>2</sub> are CHF<sub>2</sub>, CF<sub>2</sub>, CHF, CHF...HF, CF and Ng<sub>2</sub>H<sup>+</sup>.<sup>1</sup> In addition to the bands of these species, several new absorptions were found in the experimental spectra in the solid argon matrix. The new features at 613.8, 1379.4, and 1567.6 cm<sup>-1</sup> were ascribed to CF<sub>2</sub><sup>+</sup> based on comparison with calculations, and the effect of N<sub>2</sub>O (electron scavenger). All the IR active vibrations of this ion (F-C-F bending, C-F symmetric, and asymmetric modes) were identified by IR spectroscopy for the first time.

In the cases of krypton and xenon matrices, we were able to detect unusual species (FKrCF and FXeCF).<sup>2</sup> These molecules representing a new class of noble-gas compounds are presumably formed as a result of the reaction between mobile F atoms and trapped CF fragments in solid Kr and Xe, which occur after radiolysis of CH<sub>2</sub>F<sub>2</sub> in the corresponding matrices. New molecules were found to be sensitive to near-IR, visible, and UV light.

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<sup>1</sup> Sosulin, I.S.; Feldman, V.I. Radiation-induced transformations of difluoromethane in noble gas matrices, *Radiat. Phys. Chem.* **2021**, 189, 109672.

<sup>2</sup> Sosulin, I.S.; Tyurin, D.A.; Feldman, V.I. Carbene-insertion noble gas compounds: FKrCF and FXeCF, *Chem. Phys. Lett.*, **2020**, 744, 137211.