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Synthesis, Conformation, and Photochemistry of Difluoroacetyl Isocyanate $\text{CF}_2\text{HC}(\text{O})\text{NCO}$ and Isothiocyanate $\text{CF}_2\text{HC}(\text{O})\text{NCS}$

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ABSTRACT. Two carbonyl pseudohalogen compounds $\text{CF}_2\text{HC}(\text{O})\text{NCO}$ and $\text{CF}_2\text{HC}(\text{O})\text{NCS}$ have been synthesized and fully characterized by IR (gas-phase, matrix-isolation), Raman (liquid), UV-vis (gas-phase), and NMR (^{19}F , ^{13}C , ^1H) spectroscopy. The conformational properties and photochemistry of both species have been studied by combining matrix-isolation IR spectroscopy and quantum chemical calculations with the B3LYP, MPW1PW91, CBS-QB3 methods. Two conformers (*syn* and *anti*), depending on the configuration between the C=O and pseudohalogen ligands (NCO and NCS), have been unambiguously identified in both gas phase and solid noble gas matrices (Ar and Ne). Consistent with the theoretical calculations, the *syn* conformation is energetically more favorable. Upon irradiation with an ArF excimer laser (193 nm), $\text{CF}_2\text{HC}(\text{O})\text{NCO}$ and $\text{CF}_2\text{HC}(\text{O})\text{NCS}$ in cryogenic matrices eliminate CO and yield CF_2HNCO and CF_2HNCS , respectively. The underlying mechanism for the photochemistry of $\text{CF}_2\text{HC}(\text{O})\text{NCO}$ is rationalized by the elimination of the carbonyl rather than the isocyanato C=O moiety.

Keywords: Isocyanates, isothiocyanates, conformation, photochemistry, matrix-isolation, quantum chemical calculations.

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