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Synthesis, conformation, and photochemistry of difluoroacetyl isocyanate  $CF_2HC(O)NCO$  and isothiocyanate  $CF_2HC(O)NCS$ 

Ruijuan Feng, Zhuang Wu, Xiaoging Zeng

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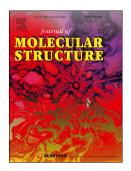
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## ACCEPTED MANUSCRIPT

Synthesis, Conformation, and Photochemistry of Difluoroacetyl

Isocyanate CF<sub>2</sub>HC(O)NCO and Isothiocyanate CF<sub>2</sub>HC(O)NCS

Ruijuan Feng, Zhuang Wu, Xiaoqing Zeng\*

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123 (China)

E-mail: xqzeng@suda.edu.cn

ABSTRACT. Two carbonyl pseudohalogen compounds CF<sub>2</sub>HC(O)NCO and CF<sub>2</sub>HC(O)NCS have been synthesized and fully characterized by IR (gas-phase, matrix-isolation), Raman (liquid), UV-vis (gas-phase), and NMR (<sup>19</sup>F, <sup>13</sup>C, <sup>1</sup>H) 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), CF<sub>2</sub>HC(O)NCO and CF<sub>2</sub>HC(O)NCS in cryogenic matrices eliminate CO and yield CF<sub>2</sub>HNCO and CF<sub>2</sub>HNCS, respectively. The underlying mechanism for the photochemistry of CF<sub>2</sub>HC(O)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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