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C and N isotope effects during UV-induced photocatalytic degradation of 2,4-dinitroanisole (DNAN) and 3-nitro-1,2,4-triazol-5-one (NTO)

CHUNLEI WANG[1], MARK E. FULLER[2], LINNEA J. HERATY[1], PAUL B. HATZINGER[2] AND NEIL C STURCHIO[1]

[1]University of Delaware

[2]Aptim Federal Services

Presenting Author: clwang@udel.edu

2,4-dinitroanisole (DNAN) and 3-nitro-1,2,4-triazol-5-one (NTO) have been used as insensitive munitions and may contaminate both surface water and groundwater environments. The biotic and abiotic transformation products (e.g. 2,4-dinitroamine, 2,4-dinitrophenol, nitrite, nitrate) of DNAN and NTO are toxic and pose a threat to environmental health. However, assessment of degradation pathways and source identification of DNAN and NTO in the environment may be difficult because the products are either unknown, common in nature (e.g., nitrite, nitrate, ammonium, N_2O), or are difficult to measure. We developed high-precision compound-specific ^{13}C and ^{15}N isotope analysis methods (^{13}C- and ^{15}N-CSIA) for DNAN and NTO (± 0.2‰) using gas chromatography-isotope ratio mass spectrometry (GC-IRMS), which enables various degradation pathways to be deciphered and identified in both laboratory and field settings. We measured normal ^{13}C fractionation (ε = -3.34‰) and inverse ^{15}N fractionation (ε = +12.30‰) of DNAN caused by photocatalytic degradation in aqueous solution under UV-A irradiation, in contrast to inverse ^{13}C fractionation (ε = +1.45‰) and normal ^{15}N fractionation (ε = -3.79‰) under UV-C irradiation [1]. Normal ^{15}N fractionation (ε = -4.84‰) and negligible ^{13}C fractionation were observed in NTO under both UV-A and UV-C irradiation. These results indicate that DNAN and NTO may act as photosensitizers and produce nitrite and nitrate during UV-induced degradation by sunlight in surface water environments and by UV-C irradation in wastewater treatment processes. Photocatalytic degradation of DNAN and NTO is demonstrated to be monitorable in aqueous systems via ^{13}C- and ^{15}N-CSIA, and it exhibits isotope effects that are distinct from those of other abiotic and enzymatic degradation pathways.

[1] C. Wang, M.E. Fuller, L.J. Heraty, P.B. Hatzinger, N.C. Sturchio, 2021. Photocatalytic mechanisms of 2,4-dinitroanisole degradation in water deciphered by C and N dual-element isotope fractionation, J. Hazard. Mater., 411.

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