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Transformation of Acetaminophen by Chlorination Produces the Toxicants 1,4-Benzoquinone and *N*-Acetyl-*p*-benzoquinone Imine

Mary Bedner* and William A. MacCrehan

Analytical Chemistry Division, National Institute of Standards and Technology, Mailstop 8392, Gaithersburg, Maryland 20899-8392

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Abstract:

The reaction of the common pain reliever acetaminophen (paracetamol, 4-acetamidophenol) with hypochlorite was investigated over time under conditions that simulate wastewater disinfection. Initially, the reaction was studied in pure water at neutral pH (7.0), a range of reaction times (2-90 min), and a molar excess of hypochlorite (2-57 times) relative to the acetaminophen concentration. The reaction was monitored using reversed-phase liquid chromatography (LC) with ultraviolet absorbance, electrochemical, and mass spectrometric detection. At 1 $\mu\text{mol/L}$ (150 ppb) and 10 $\mu\text{mol/L}$ (1.5 ppm) levels, acetaminophen readily reacted to form at least 11 discernible products, all of which exhibited greater LC retention than the parent. Two of the products were unequivocally identified as the toxic compounds 1,4-benzoquinone and *N*-acetyl-*p*-benzoquinone imine (NAPQI), which is the toxicant associated with lethality in acetaminophen overdoses. With a hypochlorite dose of 57 $\mu\text{mol/L}$ (4 ppm as Cl_2), 88% of the acetaminophen (10 $\mu\text{mol/L}$ initial) was transformed in 1 h. The two quinoidal

oxidation products 1,4-benzoquinone and NAPQI accounted for 25% and 1.5% of the initial acetaminophen concentration, respectively, at a 1 h reaction time. Other products that were identified included two ring chlorination products, chloro-4-acetamidophenol and dichloro-4-acetamidophenol, which combined were approximately 7% of the initial acetaminophen concentration at 1 h. The reaction was also studied in wastewater, where similar reactivity was noted. These results demonstrate that acetaminophen is likely to be transformed significantly during wastewater chlorination. The reactivity of the chlorine-transformation products was also studied with sulfite to simulate dechlorination, and 1,4-benzoquinone and NAPQI were completely reduced.

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