Chemical transformation of 3-bromo-2,2-bis(bromomethyl)propanol under basic conditions

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Published in: *Environmental Science and Technology 39 (2), 505-512*

ABSTRACT

The mechanism of the spontaneous decomposition of 3-bromo-2,2-bis(bromomethyl)propanol (TBNPA) and the kinetics of the reaction of the parent compound and two subsequent products were determined in aqueous solution at temperatures from 30 to 70°C and pH from 7.0 to 9.5. TBNPA is decomposed by a sequence of reactions that form 3,3-bis(bromomethyl)oxetane (BBMO), 3-bromomethyl-3-hydroxymethyloxetane (BMHMO) and 2,6-dioxaspiro[3.3]heptane (DOH), releasing one bromide ion at each stage. The pseudo-first order rate constant of the decomposition of TBNPA increases linearly with the pH. The apparent activation energy of this transformation (98±2 KJ /mol) was calculated from the change of the effective second order rate constant with temperature. The pseudo activation energies of BBMO and BMHMO were estimated to be 109 and 151 KJ /mol, respectively. Good agreement was found between the rate coefficients derived from changes in the organic molecules concentrations and those determined from the changes in the Br^- concentrations. TBNPA is the most abundant semi-volatile organic pollutant in the aquitard studied, and together with its by-products they poses an environmental hazard. TBNPA half-life is estimated to be about 100 years. This implies that high concentrations of TBNPA will persist in the aquifer long after the elimination of all its sources.

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