Chemical degradation of 2,2-bis(bromomethyl)-propan-1,3-diol (DBNPG) in alkaline conditions

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ABSTRACT

The mechanism and kinetics of the spontaneous decomposition of 2,2-bis(bromomethyl)propan-1,3-diol (DBNPG) and its decomposition daughter products were determined in aqueous solution at a temperatures range between 30 19 and 70°C and pH from 7.0 to 9.5. DBNPG decomposition in basic aqueous solutions involves release of bromide ions through a sequential formation of 3-bromomethyl-3-hydroxymethyloxetane (BMHMO) and 2,6-dioxaspiro[3.3]heptane (DOH). DBNPG decomposition into BMHMO is a two stage reaction. The first stage is an acid/base equilibrium, in which an alkoxide is formed. In the second stage, DBNPG predominantly undergoes an intramolecular nucleophilic substitution to form the BMHMO. The transformation rate increases with the pH and the energy barrier for
the degradation is 98 kJ mol$^{-1}$. Good agreement was found between the rate coefficients derived from variations in the organic molecules concentrations and those determined from the changes in the Br$^{-}$ concentration. DBNPG is one of the most abundant pollutants in a studied polluted aquitard underneath industrial park in the northern Negev, Israel, and together with its by-products pose an environmental hazard. DBNPG half-life is estimated to be about 65 years. This implies that high concentrations of DBNPG will persist in the aquifer long after the elimination of all its sources.

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