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Aminohydroxypropane Esters of Hydroxyethylidenebisphosphonic Acid

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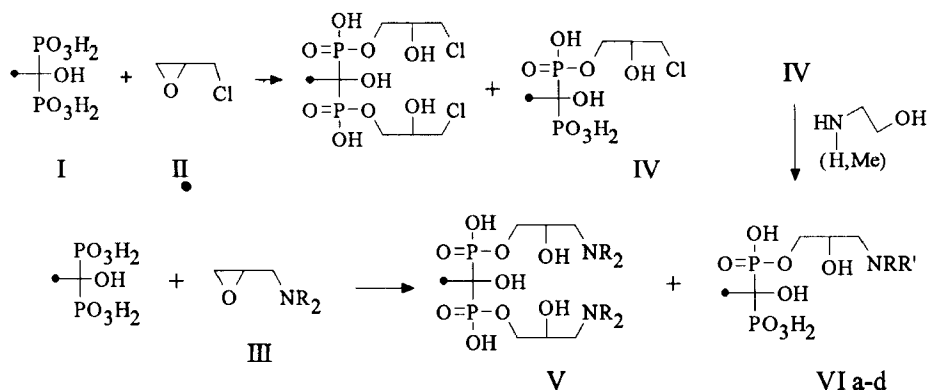
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AMINOHYDROXYPROPANE ESTERS OF HYDROXYETHYLIDENEBISPHOSPHONIC ACID.

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The 1-hydroxyethylidene-1,1-bisphosphonic acid (HEDP) (I) reacts with epichlorohydrine (II) and aminoepoxypropanes (III) in water. Optimum pH for the esterefication is 6-7. The reaction completes in 20-30 h on 60°C at this pH and leads to the mixture of the original HEDP with the mono- and diesters. The mixture of di-Na salts of HEDP and the monochloroester (IV) in ratio 1:1.7 was precipitated from the reaction solution on using of the epichlorohydrine (II). This mixture was used for synthesis of aminoesters (VI a,b) unavailable by direct reaction of HEDP with corresponding aminoepoxides.



VI) RR' = H, C₂H₄OH (a), Me, C₂H₄OH (b), (C₂H₄)₂O (c), Et₂ (d).

The aminoesters (V, VI) was isolated by ion-exchange chromatography on KU-2-8 (analog Dowex-50X8) ion-exchange resin.

Obtained aminoesters (V and VI) are glassy or crystalline hygroscopic substances. Any precipitate doesn't appear in the water solution of (VI) when Ca²⁺ salts are added.

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