SHORT COMMUNICATIONS

A New Chelating Agent, α, α'-Diamino-*o*-xylene-*N*, *N*, *N'*, *N'*-tetraacetic Acid

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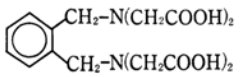
A large number of ethylenediaminetetraacetic acid (EDTA) derivatives have been known in the literatures, and it is therefore, possible to study the influence of electronic and steric variations on their chelating behaviors toward metal ions. However not many informations are available about the EDTA derivatives containing the benzene ring. We are now successful to synthesize α, α'-diamino-*o*-xylene-*N*, *N*, *N'*, *N'*-tetraacetic acid, (*o*-XyDTA) which is a new complexane containing benzene ring.



The tetramethyl ester of this acid was prepared by the condensation of α, α'-dibromo-*o*-xylene (0.01 mol.) with iminodiacetic acid dimethyl ester (0.06 mol.) in dry acetone at 70—80°C, with refluxing for 8 hr. After the reaction, the precipitated iminodiacetic acid dimethyl ester hydrobromide was filtered off and the crude tetra ester was obtained from the filtrate after distilling off acetone under reduced pressure. The ester was hydrolyzed with 10% sodium hydroxide at 70°C for 8 hours. After cooling, the pH of the solution was adjusted to about 1. The precipitated crude acid was recrystallized from hot water: yield about 20%. It decomposed at 226—229°C.

Found: C, 52.27; H, 5.53; N, 7.64%.[1] Calcd. for $C_{16}H_{20}N_2O_8$: C, 52.17; H, 5.53; N, 7.64%.

Pure acid is slightly soluble in water (about 0.4 g./1000 ml. H_2O).

The acid dissociation constants were determined by the potentiometric method at 25°C, in a medium of ionic strength of 0.10, with sodium hydroxide as a titrant. The titration curve is essentially the same as that of EDTA. The constants of this acid were calculated by the method of Schwarzenbach et al.[2] except that an algebraic method of solution was used instead of a graphical one. The results are $pk_1=2.0$: $pk_2=2.71$: $pk_3=5.99$: $pk_4=10.88$. The values of k_1, k_2, k_3 are similar to those of EDTA, but k_4 is fairly less than EDTA.

This acid showed similar chelating behavior to EDTA on the qualitative test using metal indicators such as Erio T (pH 10, Ca, Mg) or xylenol Orange (pH 5—6, Zn).

The chelating behavior toward metal ions in aqueous solution is now under study. The results of the detailed investigation on this ligand will be published later.

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1) Elementary analysis was carried out at the Service Center of Elementary Analysis of Organic Compounds of Kyushu University.

2) G. Schwarzenbach, A. Willi and R. O. Bach, *Helv. Chim. Acta*, **30**, 1303 (1947).