Supporting Information

Electrolysis of Trichloromethylated Organic Compounds under Aerobic Conditions Catalyzed by B₁₂ Model Complex for Ester and Amide Formations

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Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Motooka, Fukuoka 819-0395, Japan. E-mail: shimakoshi@mail.cstm.kyushu-u.ac.jp; yhisatcm@mail.cstm.kyushuu.ac.jp;Fax: +81-92-802-2828; +81-92-802-2828 Electrolysis of 1,1,2,2-tetrachloro-1,2-diphenylethane (4) catalyzed by B₁₂ model complex (1).



The controlled-potential electrolysis of 1,1,2,2-tetrachloro-1,2-diphenylethane (4) was carried out in a one-compartment cell equipped with a Pt mesh cathode and a zinc plate anode $(1x3 \text{ cm}^2)$ at -0.9 V *vs*. Ag/AgCl in the presence of **1** at room temperature in 0.1 M *n*-Bu₄NClO₄ containing ethanol under N₂. The zinc electrode was used as a sacrificial anode. The applied potential between the working and reference electrodes in the electrolysis was maintained constant using a Hokuto Denko HA BF-501A potentiostat, and the electrical quantity was also recorded by it. The concentrations of the catalyst and substrate were $5.0x10^{-4}$ M and $5.0x10^{-3}$ M, respectively. After the electrolysis, the electrolyte solution was passed through in silica gel with CHCl₃ eluent, then analyzed by GC-MS. Conversion of **4**: 77%, yields of **5a**: 11%, yields of **5b**: 47%.



Figure S1. UV-vis absorption spectrum of mercury (II) thiocyanate reagent with aerobic electrolysis solution.

Wavelength / nm



Figure S2. ESR spectra observed during the electrolysis at -0.9 V vs. Ag/AgCl in C_2H_5OH ; [1]=5x10⁻⁴ M; [4-chloro-benzotrichloride]=5.0x10⁻² M; [DMPO]=2.5x10⁻¹ M; [*n*-Bu₄NClO₄]=1x10⁻¹ M under N₂ (a) and air (b).

substrate



Figure S3. (a) GS-MS of B_{12} model complex (1) catalyzed reaction mixture after a 1h electrolysis in CH₃CN under air, (b) mass pattern of RT=11.4 min. peak.



Figure S4. UV-vis spectral changes during electrolysis at -0.9 V vs. Ag/AgCl under N₂: [1]= $3.2x10^{-4}$ M, [benzotrichloride]= $3.2x10^{-2}$ M, [*n*-Bu₄NClO₄]= $1x10^{-1}$ M in C₂H₅OH.