Supporting Information

Chemical Fixation of Carbon Dioxide by NaI/PPh₃/PhOH

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Experimental Section.

General Methods. Melting points are uncorrected. ¹H, ¹³C and ³¹P NMR spectra data were recorded at 300, 75 MHz and 121 MHz, respectively. Mass and HRMS spectra were recorded by EI methods. Organic solvents used were dried by standard methods when necessary. All solid compounds reported in this paper gave satisfactory CHN microanalyses. Commercially obtained reagents were used without further purification.

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^{13}C NMR spectrum of **1e**.

The deuterium labeling experiment

Determination of β -hydroxy phosphonium salt **4**

^1H NMR spectrum of β -hydroxy phosphonium salt **4**.

¹³C NMR spectrum of β-hydroxy phosphonium salt 4.

DEPT spectrum of β -hydroxy phosphonium salt **4**.

H H-COSY spectrum of β -hydroxy phosphonium salt **4**.

HMQC spectra spectrum of β -hydroxy phosphonium salt **4**.

HMBC spectrum of β -hydroxy phosphonium salt **4**.

The determination of the structure for β -hydroxy phosphonium salt **4**.

^{31}P NMR showed the presence of a phosphine atom. In the ^1H -NMR spectrum, the presence of a hydroxylic hydrogen was confirmed by D_2O exchange experiments and the other twenty one protons were assigned as a triphenylphosphine and an $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2$ segment, respectively, through ^{13}C -NMR, DEPT, HH-COSY, and HMQC. In the HMBC spectra, the quaternary carbon at 118.56 (d, $J_{\text{C-P}} = 86.4$ Hz, C) showed a long distance correlation with two methylene protons at 3.46 (ddd, $J = 15.3, 12.6, 2.7$ Hz, 1H, CH_2), 3.81 (ddd, $J = 21.0, 15.3, 10.5$ Hz, 1H, CH_2), which suggested that triphenylphosphine was connected to $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2$ group. Considering the elemental analyses (Anal. Calcd. For $\text{C}_{21}\text{H}_{22}\text{IOP}$: C, 56.27; H, 4.95; I, 28.31. found: C, 55.83; H, 5.19; I, 28.14%), its chemical structure was determined as a iodide salt of 1-(triphenyl- λ^5 -phosphanyl)-propan-2-ol **4**. mp. 119-121 $^\circ\text{C}$; IR (Neat): ν 3311, 1588, 1485, 1438, 1112 cm^{-1} ; ^1H NMR (CDCl_3 , TMS, 300 MHz): δ 1.51 (dd, $J = 5.7, 2.4$ Hz, 3H, CH_3), 3.46 (ddd, $J = 15.3, 12.6, 2.7$ Hz, 1H, CH_2), 3.81 (ddd, $J = 21.0, 15.3, 10.5$ Hz, 1H, CH_2), 4.05 (d, $J = 6.6$ Hz, OH), 4.20-4.33 (m, 1H, CH), 7.64-7.83 (m, 15H). ^{13}C NMR (75 MHz, CDCl_3 , TMS): δ 25.5 (d, $J_{\text{C-P}} = 14.0$ Hz, CH_3), 32.6 (d, $J_{\text{C-P}} = 51.4$ Hz, CH_2), 62.7 (d, $J_{\text{C-P}} = 6.2$ Hz, CH), 118.6 (d, $J_{\text{C-P}} = 86.4$ Hz, C), 130.1 (d, $J_{\text{C-P}} = 12.6$ Hz, CH), 133.9 (d, $J_{\text{C-P}} = 10.4$ Hz, CH), 134.7 (d, $J_{\text{C-P}} = 2.8$ Hz, CH). Anal. Calcd. For $\text{C}_{21}\text{H}_{22}\text{IOP}$: C, 56.27; H, 4.95; I, 28.31. found: C, 55.83; H, 5.19; I, 28.14%.