

## Fullerene Hydride - A Potential Hydrogen Storage Material

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Hydrogen, as a clean, convenient, versatile fuel source, is considered to be an ideal energy carrier in the foreseeable future. Hydrogen storage must be solved in using of hydrogen energy. To date, much effort has been put into storage of hydrogen including physical storage via compression or liquefaction, chemical storage in hydrogen carriers, metal hydrides and gas-on-solid adsorption [1]. But no one satisfies all of the efficiency, size, weight, cost and safety requirements for transportation or utility use.

$C_{60}H_{36}$ , firstly synthesized by the method of the Birch reduction [2], was loaded with 4.8 w.t.% hydrogen indicating  $C_{60}H_{36}$  fullerene might be a potential hydrogen storage material. If a 100% conversion of  $C_{60}H_{36}$  is achieved, 18 mols of  $H_2$  gas would be liberated from each mole of fullerene hydride. Pure  $C_{60}H_{36}$  is very stable below 500°C under nitrogen atmosphere and it releases hydrogen according to other hydrocarbons under high temperature [3]. But  $C_{60}H_{36}$  cannot be decomposed to generate  $H_2$  under effective catalyst.

We have reported that hydrogen can be produced catalytically from  $C_{60}H_{36}$  by Vaska's compound ( $IrCl(CO)(PPh_3)_2$ ) under mild conditions [4].  $RhCl(CO)(PPh_3)_2$  having similar structure to  $IrCl(CO)(PPh_3)_2$ , was also examined for thermal dehydrogenation of  $C_{60}H_{36}$ ; but it showed low catalytic activity.

To search better catalyst, Palladium carbon (Pd/C) and Platinum carbon (Pt/C) catalysts, which were known for catalytic hydrogenation of aromatic compounds, were tried and good results were obtained. A very big peak of hydrogen appeared at  $\delta$  5.2 ppm in the  $^1H$  NMR spectrum based on Evans' work [5] (fig.1) at 100°C over a Pd/C catalyst for 16 h. It is shown that hydrogen produced from  $C_{60}H_{36}$  using a catalytic amount of Pd/C. Comparison with Pd/C

Pt/C catalyst showed lower catalytic activity.

The high cost and limited availability of expensive catalysts for our process based on Pt/C were used as a catalyst in our experiments. Over a Ni-Al alloy catalyst for 20 h showed

Vaska's compounds, Pd and Pt are more expensive than on-precious metals. Very cheap Ni-Al alloy catalysts are more advantageous to develop less expensive catalysts (containing 40.50% of Ni). A big peak of hydrogen at  $\delta$  5.6 ppm in the  $^1H$  NMR spectrum (fig.2) at 100°C over a Ni-Al alloy catalyst for 20 h showed

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Fig. 1. The  $^1H$  NMR spectrum of catalytic dehydrogenation of  $C_{60}H_{36}$  (20 mg) in 0.5 ml of  $ODCB-d_4$ , Pd/C (15 mg), 100°C, 16 h.

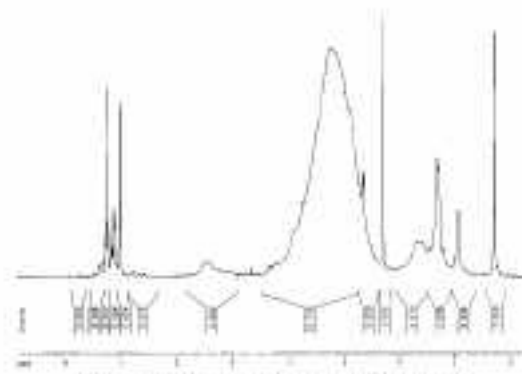


Fig. 2. The  $^1H$  NMR spectrum of catalytic dehydrogenation of  $C_{60}H_{36}$  (20 mg) in 0.5 ml of  $ODCB-d_4$ , Ni-Al Alloy (15 mg), 100°C, 20 h.

To measure the amount of hydrogen decomposed from  $C_{60}H_{36}$ , we developed a cylindrical reactor based on Pomesic's work [6] and determined it by GC. The amounts of hydrogen produced from 100 mg of  $C_{60}H_{36}$  at 100°C for 16 h were 0.78 mmol (17.47 ml) and 0.52 mmol (11.73 ml) with decompose ratio of 33% and 22% for 50 mg of Pd/C catalyst and 50 mg of  $IrCl(CO)(PPh_3)_2$  catalyst, respectively.

In summary, fullerene hydride, which can produce hydrogen over effective catalysts, may be a potential hydrogen storage material in future.

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[1] A. Züttel, *Mater. Today* 9, 24, 2003.

[2] R. E. Haufer *et al.*, *J. Phys. Chem.* 94, 8634, 1990.

[3] A. A. Peera, L. B. Alemany, W. E. Billups, *Appl. Phys. Lett.* 76, 1004, 1999.

[4] N.-X. Wang *et al.*, *Tetrahedron Lett.* 42, 7911, 2001.

[5] D. F. Evans, *Chem. Ind.* 1960, 1961.