CHAPTER 4

RESULLTS AND DISCUSSION

4.1 Synthesis of tetrahexyltin by Grignard reaction.

The reactants and the solvents had to be absolutely dry and the humidity had to be totally excluded from the reaction medium by dean-stark apparatus.

This synthesis was modified by replacing the solvent, THF, with toluene after the Grignard reagent had been synthesized and allowed the Grignard reagent to react with stannic chloride in dried toluene. This increased the yield of the product and prevent the solid formation of a stannic chloride-THF complex, which would otherwise clog the dropping funnel. It was believed that the product yield increased due to the solubility of stannic chloride in dried toluene was better than THF and ether (22,23), otherwise, toluene had much higher boiling point than THF and ether and did not form the solid complex with stannic chloride. In this study the result product was 91.06% yield based on stannic-chloride.

Characteristics of tetrahexyltin ($(C_6H_{13})_4Sn$) were confirmed by ^{13}C NMR and Mass Spectrometer.

^{13}C NMR showed the peak of CH_3- at 14.193 ppm, $-CH_2-$ at 22.861,27.141,31.692 and 34.346 ppm, respectively.

The peak of CH_2-Sn appeared at 9.263 ppm.

Mass Spectrum showed base peak at 375 and m-85/e at 373 due to it lost C_6H_{13} as following equation:

$$(C_6H_{13})_4Sn \text{ ---------> } (C_6H_{13})_3Sn^+ + C_6H_{13}^-$$

M.W. 373 M.W. 85

4.2 Antiknock properties of tetrahexyltin, iso-propyl and iso-butyl alcohols.

Tetrahexyltin was prepared and tested for their antiknock properties in gasoline engine both with and without alcohols. This compound was selected on the basis of its stability and its solubility in gasoline. In this study the data were taken from the sample with tin content 1g Sn and 2g Sn, and alcohol content 5%, 7% and 10% for the acceptable range of practical blends. Results from octane number determinations of gasoline composition base mixed with tetrahexyltin and alcohols showed that they had antiknock property both low octane gasoline composition and high octane gasoline composition in various concentrations of tin and alcohols.

Fig 3.5 and table 3.1 depicted that the RON data for gasoline composition mixed with tetrahexyltin and iso-propyl alcohol (IPA). The observed data showed that the gasoline composition containing 1g Sn and 2g Sn made higher octane number than gasoline composition base by 1.2 and 1.4 units, the gasoline composition containing 5%, 7%, 10% IPA increased octane number by 1.4, 2.3, 3.9 units respectively which were compared with gasoline composition base. As the gasoline composition base was mixed with tetrahexyltin and IPA, to compare with gasoline composition base, the octane number increased by 2 - 5.1 units.

Fig 3.6 and table 3.2 presented that the RON data for gasoline composition containing tetrahexyltin and iso-butyl alcohol (IBA). These experimental data demonstrated that gasoline composition which contained 1g Sn and 2g Sn added octane number by 1.2 and 1.9 units in comparison with gasoline composition base. When 5%, 7%, 10% IBA were added in gasoline composition base, differences of the octane number between gasoline composition containing 5%, 7%, 10% IBA and gasoline composition base were 2.4, 2.8, 3.8 units respectively. After tin and alcohol were blended together with gasoline composition, the octane number increased by 3.2-4.8 units in comparison with gasoline composition base.

Fig 3.7 and table 3.3 showed that the RON data for the blends of gasoline composition with tetrahexyltin and alcohols (IPA:IBA; 50:50). We found that gasoline composition which contained 1g Sn and 2g Sn improved octane number which compared with gasoline composition base by 1.1 and 1.4 unit. The observed octane number of gasoline composition mixed with alcohols increased by 1.7, 2.6, 3.6 units respectively by comparing with gasoline composition base. After tin and alcohols were blended together, the observed octane number increased by 2.5-5 units when comparing with gasoline composition base.

Fig 3.8 and table 3.4 illustrated that the RON data for the mixing of gasoline composition with tetrahexyltin and IBA at high octane number. From these remarked results, when 1g Sn and

2g Sn were added in gasoline composition base, the octane number, by comparing with gasoline composition base, advanced by 0.5 and 0.9 units. After tin and alcohol were blended together, the octane number which compared with gasoline composition base increased by 1.9-3.5 units.

The data of MON rating and RON rating in table 3.1-3.4 showed that the sensitivities of fuel were in the range of 4-8 units.

From these experimental results indicated that the octane numbers of gasoline composition blended with 1g Sn were resembled the octane numbers of gasoline composition mixed with 2g Sn in increments. The gasoline composition with large concentration of alcohol produced greater increases in RON rating than small concentration. The gasoline composition which blended with mixed alcohols increased in RON rating more smoothly than using alcohol alone and the octane number was between IPA and IBA, see fig 4.1. The sensitivities of fuel showed that the performances of fuel were acceptable due to RON and MON were not spaced very much (4-8 units).

4.3 Other properties of iso-propyl and iso-butyl alcohols

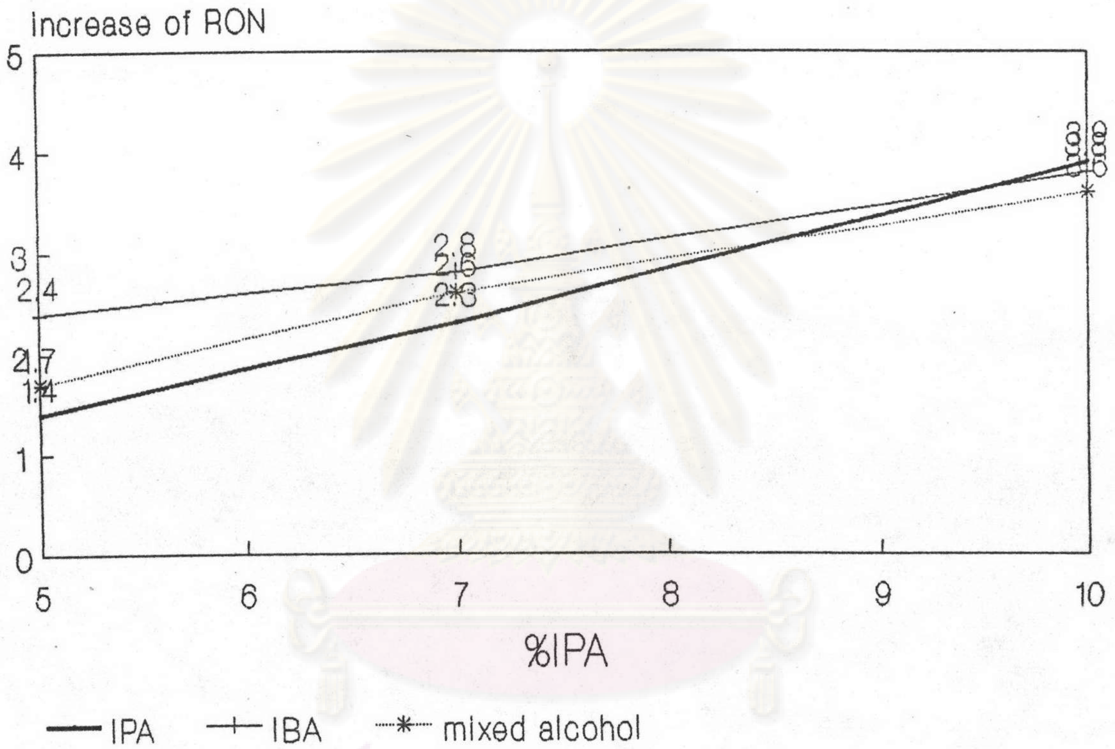
The determination of volatility were tested through distillation and Reid Vapour Pressure.

Results from distillation of gasoline composition base blended with alcohols demonstrated that they volatiled in the ASTM standard.

Results from Reid Vapour Pressure of gasoline composition mixed with alcohols showed that RVP were quite

FIG 4.1

Increase of RON vs. conc. of alcohols.



low because the preparation spent a lot of time before tested and made the light composition lose.

Determination of copper corrosion showed that the blends of gasoline composition and alcohol had the least corrosiveness. (No.1)

The gum contents in gasoline composition containing alcohols were checked and reported that the gum contents were not more than 1 mg/100 ml.

Heating value of gasoline composition was more than gasoline composition mixed with alcohol and increased when the mass was reduced. However, heating value of gasoline composition mixed with alcohols were increased upto 7% alcohol and then dropped a little. These experimental data indicated that the optimum of heating value was 7% alcohol.

All of the tested properties showed that the gasoline composition containing alcohols volatiled quite well, had a little corrosion, good stability.

A comparison of antiknock property improvement of tetrahexyltin mixed with alcohols and MTBE was found that 10% alcohol mixed with 2g Sn could be improved the RON by 5 units corresponding to 15% MTBE (10). But the cost of alcohols was much cheaper than MTBE and organotin compound could be synthesized by the use of tin which had very much in Thailand to decrease the cost of synthesis. For these reasons, alcohols and organotin compound should be interesting to replace MTBE.