Synthesis of Bis-(borane diisopropylphosphino) Methyl Calcium a Novelty Carbanion System

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1. Introduction:

Why is carbanion system a novelty?

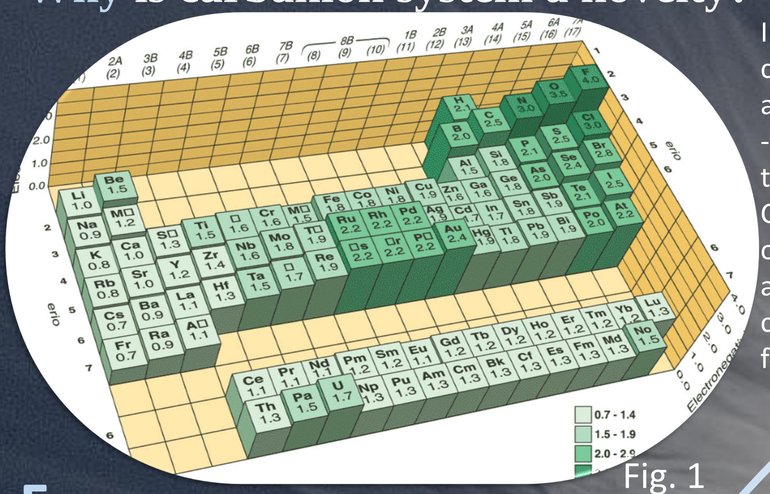


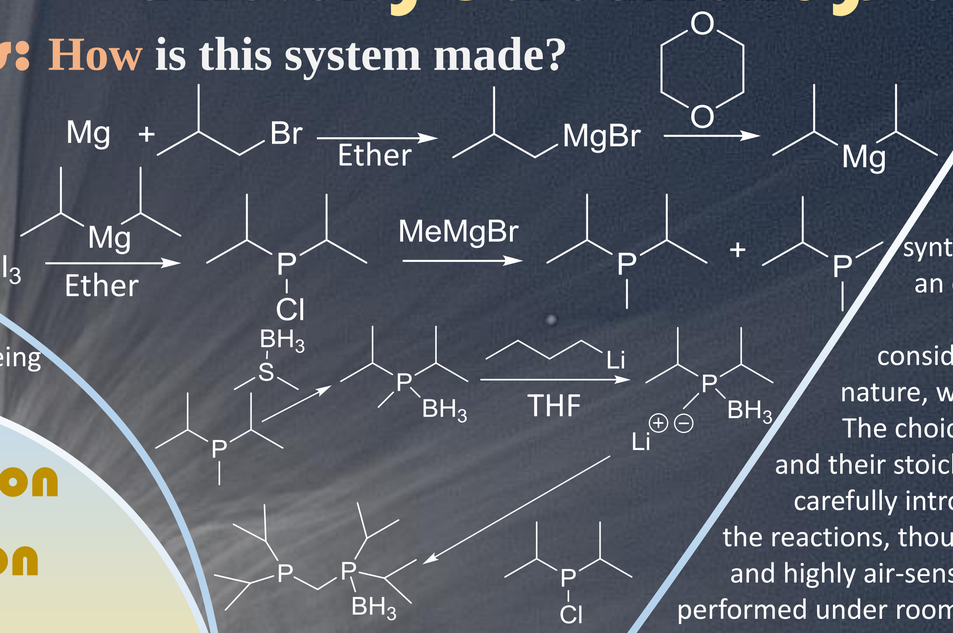
Fig. 1
Electronegativity of elements.

In the field of chemistry, It is generally agreed that the more electro--negative an element is, the more likely this element will ad0pt negative oxidation states. Carbon, being a light atom with electronegativity of 2.5, is regarded as possessing limited potential of being a carbon anion, carbanion for short.

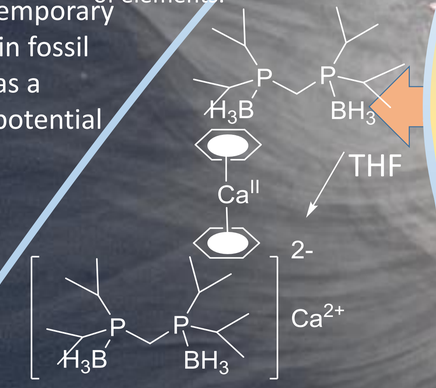
For centuries, carbon, from it's original meaning of "coal" in Latin to the contemporary understanding of its vital significance in fossil fuels and biology, has been regarded as a fundamental element with immense potential in synthesis.

However, with centuries of research, unanswered questions regarding the chemistry of carbon still persist. What oxidation states, apart from +2, +3 and +4, can carbon adopt? Can it ever adopt oxidation states of -1, or even -2? The answer lies within electronegativity. As Fig. 1 illustrates, the height of the "block of element" represents the correspondent electro--negativity.

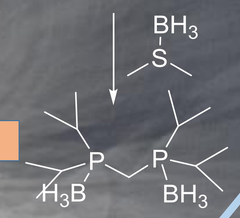
2. Reaction schemes: How is this system made?



The ten-step synthesis provided an overall yield of 5.07%, which, considering its linear nature, was acceptable. The choices of reagents and their stoichiometry were carefully introduced so that the reactions, though exothermic and highly air-sensitive, could be performed under room temperature.



Scheme 1.2



Scheme 1.1

4. Conclusion & Evaluation

The Synthesis route has yielded the target product, but impurities, as you can see in Fig. 4, are still present. This outcome indicates the success of the design and execution of an unprecedented synthesis route, while encouraging further research for improvements and modifications.

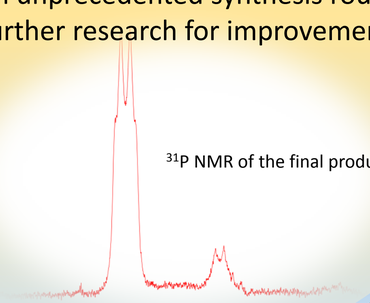


Fig. 4

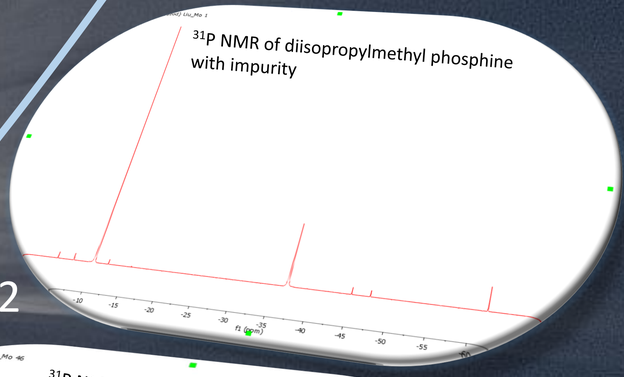


Fig. 2

3. Obstructions & Solutions:

During the synthesis, the issue of purification had become particularly troublesome. As you can see in Fig. 2.1, the NMR spectrum indicates that instead of one pure compound, the synthesis route of diisopropyl methyl phosphine resulted in a mixture of two compounds: the ever so desired phosphine and an unwanted impurity.

The mixture proved itself extremely challenging to separate as chemistry requires previous data to be properly performed. Given the fact that the entire system was unprecedented, was painfully limited. In this case, a game of " trail and error" was in order. After weeks of planning, attempting and failing, the target material, diisopropyl methyl phosphine, was finally distilled from its foul surrounding at 68-74 degrees Celsius, 150 mBar (Fig. 2.2). This piece of data was condensed from all the time and effort devoted to this research. That being said, **the true cause of impurities remains unknown.**

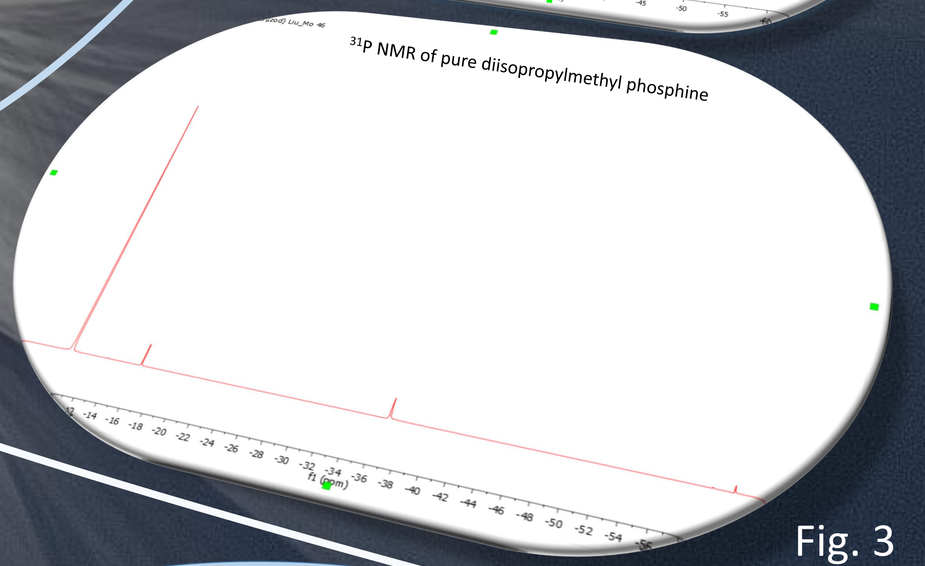


Fig. 3

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References:

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