**Reversible, Metal-Free Hydrogen Activation**

Welch, G. C.; San Juan R. R.; Masuda, J. D.; Stephan, D. W. *Science* **2006**, *314*, 1124–1126

This literature discussion was written in Spring 2022 to celebrate Professor Douglas W. Stephan, the recipient of the F. Albert Cotton Award in Synthetic Inorganic Chemistry.

**Questions**

1. The article reports a pathway for hydrogen activation using an usual phosphonium borate molecule. Please briefly summarize and provide the significances of this article on this hydrogen activation.
2. The synthesized compound **3** consists of both Lewis acid and Lewis base sites in the same molecule. Because of this feature, this compound was later classified as frustrated Lewis pairs.1 Please identify these Lewis acid and the Lewis base sites, and provide a brief explanation to support your answers.
3. Explain why B(C6F5)3 and PH(C6H2Me3)2 undergoes a para-nucleophilic aromatic substitution reaction to form product **1**, instead of the expected acid-base reaction. Please draw a chemical structure of what could have been a product from the acid-base reaction.
4. Compound **1** is reported to be air and moisture stable. Please provide a possible explanation for the high stability of this compound.
5. Please use the information provided below on the chemical shifts of signals to sketch a qualitative 19F{1H}NMR spectrum of compound **2**. Be sure to draw each signal with the correct splitting pattern. You may use a tree splitting diagram to identify the splitting pattern of each signal. 19F is 100% natural abundant with the nuclear spin I = 1/2.

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| **Chemical shifts (ppm)** | **F atoms** | **Integrations** |
| –127.52 | C6F4 | 2 |
| –134.09 | *Ortho*-C6F5 | 4 |
| –134.95 | C6F4 | 2 |
| –163.87 | *Para*-C6F5 | 2 |
| –167.43 | *Meta*-C6F5 | 4 |

1. Provide two experimental evidence for the loss of hydrogen gas from compound **2** to form compound **3**.
2. Sketch chemical schemes and list the key reaction intermediates for the H/D scrambling reactions that lead to the formation of compounds **2**, **2-d2**, **2dP**, and **2dB** from heating of compound **2-dB**or **2-dP**. No curved arrows are required.
3. The enthalpy and the entropy of activation of the generation of **3** from **2** were reported to be 90 kJ/mol and –96 J/K·mol, respectively. Please perform any necessary calculations by using the Eyring Plot found in the Supporting Online Material to confirm these reported values.

**Reference**:

1. McCahill, J. S. J.; Welch G. C.; Stephan D. W. *Angew. Chem. Int. Ed.* **2007**, *46*, 4968–4971.