

Discussion of (the) Room-temperature chemical synthesis of dicarbon – open and transparent science.

Henry Rzepa 

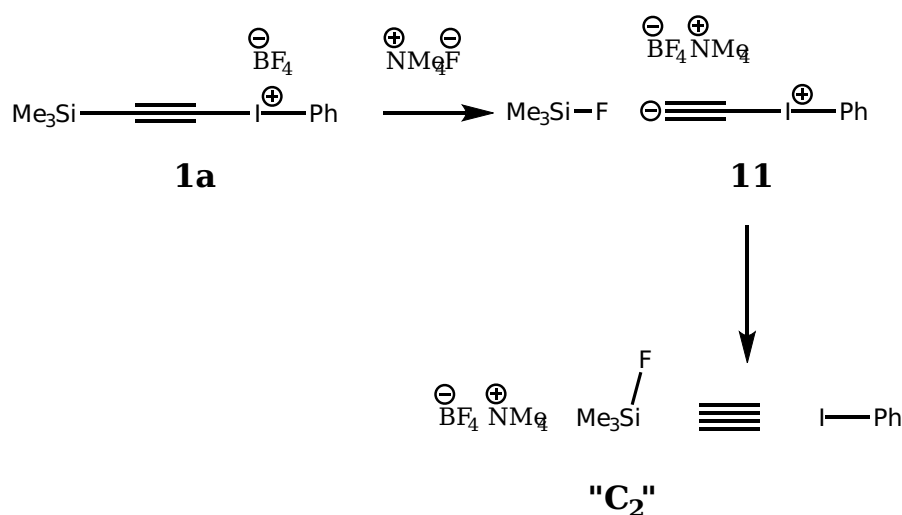
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Keywords

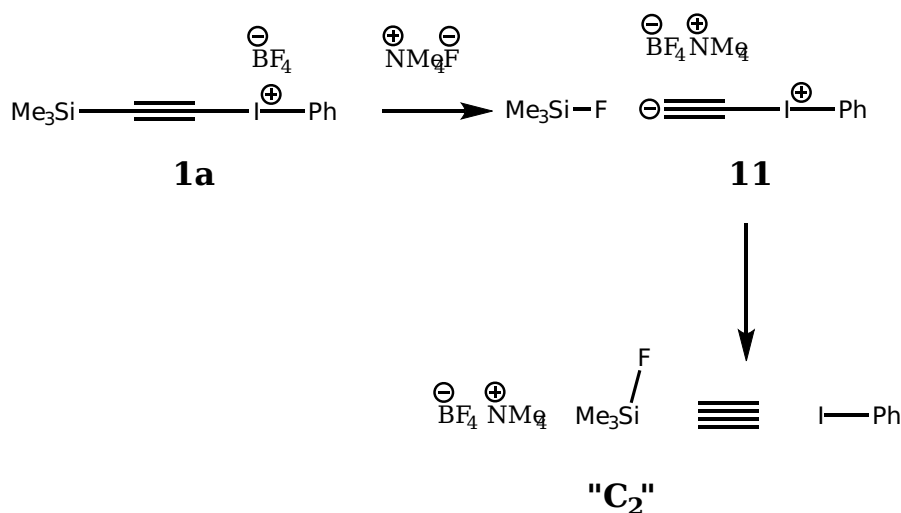
Interesting Chemistry, Reaction Mechanism



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A little more than a year ago, a ChemRxiv pre-print appeared bearing the title referenced in this post,[\[cite\]10.26434/chemrxiv.8009633.v1\[/cite\]](#) which immediately piqued my curiosity. The report presented persuasive evidence, in the form of trapping experiments, that dicarbon or C₂ had been formed by the following chemical synthesis. Here I describe some of what happened next, since it perhaps gives some insight into the processes of bringing a scientific result into the open.



My curiosity at that time was because a thermal facile reaction is normally associated with a sufficiently low free energy barrier to the transition state to allow a flux of the product to form on a reasonable timescale, and at a concentration that can be *e.g.* trapped. Dicarbon however is normally considered a very high energy species. Its formation from a precursor bearing a triple bond in this case would involve breaking the $\text{C}\equiv\text{C}-\text{I}$ bond in **11** above and replacing it by C-C, where the 4th bond is experimentally estimated to recover ~20 kcal/mol of energy. I estimated the bond dissociation energies and further calculated the free energies of the reactions of **1a**, **11** and "C₂" above, thus adding to the information available from the pre-print.

The original pre-print has now appeared as a full paper in *Nature Communications*, having passed through the peer review processes.[\[cite\]10.1038/s41467-020-16025-x\[/cite\]](#) I can reveal here that I was one of the referees of this article. In my referee report I felt it appropriate to comment on my thermochemical observations on the reaction. I also waived my anonymity as part of this process (an option given to referees of this journal). Regarding the thermochemistry as essential to understanding this fascinating reaction and because it is not discussed in the final published article itself,[\[cite\]10.1038/s41467-020-16025-x\[/cite\]](#) I decided to add this to the public record in the form of a matter arising (MA), also submitted to *Nature Communications*. Interestingly, such a form of response incurs no open access article processing charge (APC), unlike the communications themselves. In its acknowledgement of submission, the journal informs the submitting author that they can freely place the final author-version of the submission onto a pre-print server.[‡] In a sense, this completes the first cycle of this process, since that is how it all started a year ago.[\[cite\]10.26434/chemrxiv.8009633.v1\[/cite\]](#) Accordingly, you can now judge my case for the thermochemistry[\[cite\]10.26434/chemrxiv.12237980\[/cite\]](#) as a ChemRxiv pre-print. This is not yet the end of the process, since the MA itself is now subjected

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to peer review and the original authors can also respond, a process that can take several months.

Until recently, the mechanisms by which any given scientific article emerges, fully formed so to speak, into the (possibly) open *via* a journal has tended towards opaqueness, with much of the process of assessment shrouded in anonymity. At a time of a global epidemic, with major life changing daily decisions being (hopefully) made on the basis of [scientific discussion and \(open?\) evidence](#), it is I think especially pertinent to show how science can operate openly and transparently, to some extent and on occasion at least.

‡I was informed by the editor of the journal that a blog such as this can also be considered an appropriate pre-print server. Perhaps it was a sense of symmetry that made me chose the same location where this story started, whilst charting its progress here.

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