

Abstract:

This research explores the synthesis of sulfonium ylides as carbene precursor molecules. A carbene is a highly reactive molecule containing a neutral carbon atom with two nonbonded electrons and two substituents. Due to their unique reactivity, carbenes are important in chemistry because they play key roles in catalysis, organic synthesis, and material science. As part of a proposed five-step synthesis to generate sulfonium ylide precursor molecules, α,β -unsaturated ketone 1-(4-bromophenyl)-3-(4-bromophenyl)prop-2-en-1-one was synthesized, as evidenced by ^1H NMR spectroscopy. Further modification of this molecule via oxidation was attempted; however, despite exploring multiple routes, including hydrolysis, epoxidation, and oxidation, success was not achieved, and an alternate synthetic route was proposed. This research provides valuable insights into carbene precursor synthesis, particularly in understanding carbon-based compound formation essential for life and beneficial for modern material synthesis.

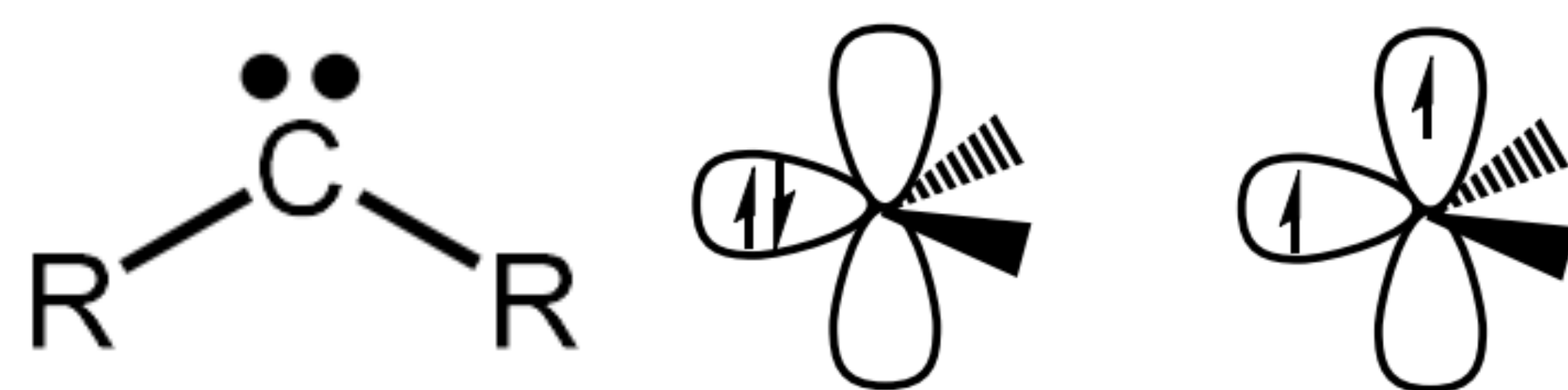


Figure 1. Carbene intermediate (left) with singlet (center) and triplet (right) electronic states.

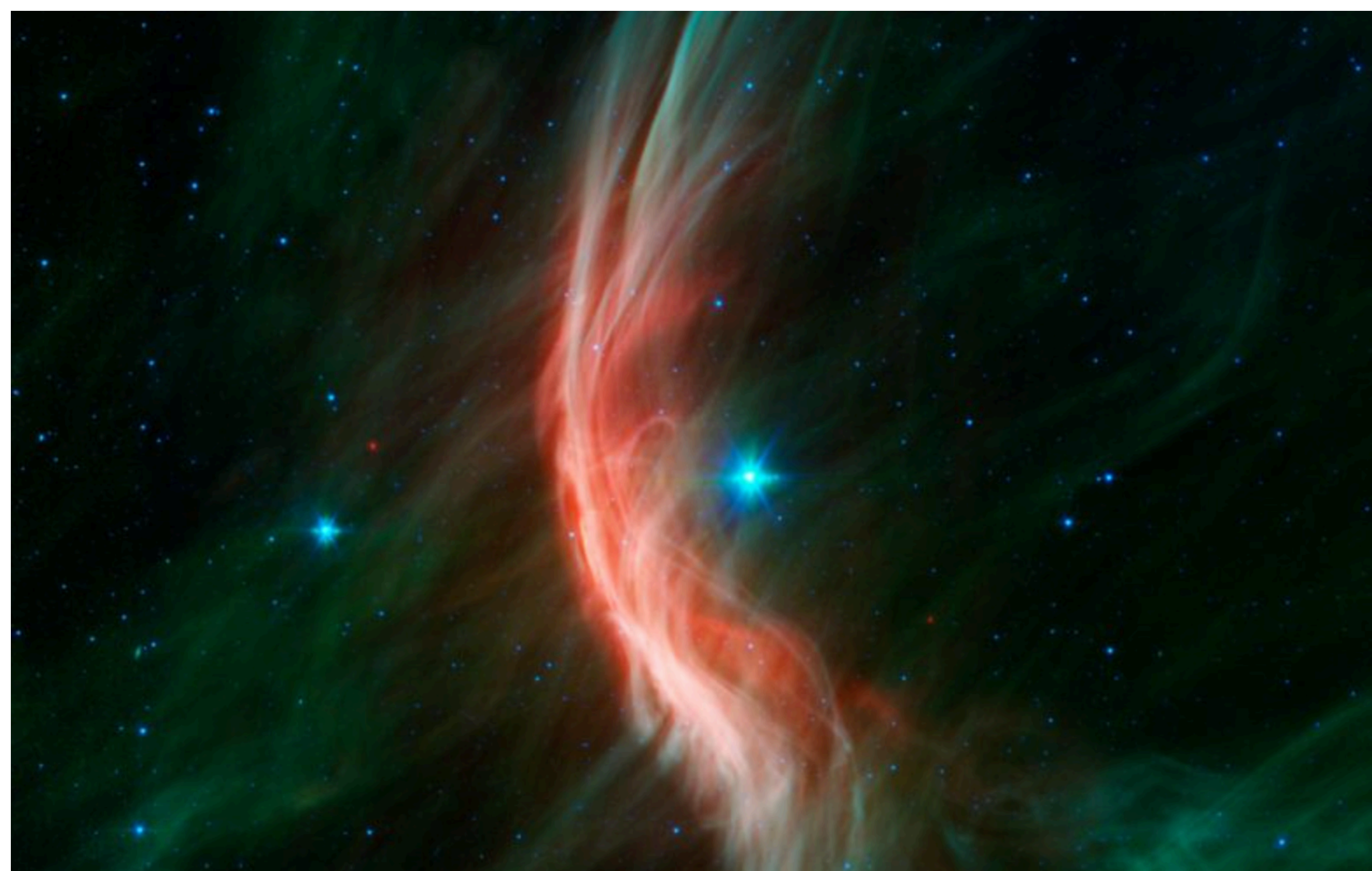
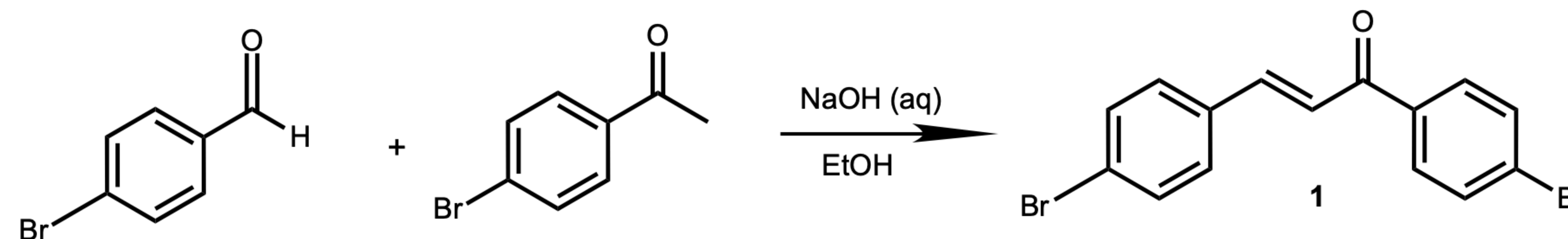


Image 1. Carbene compounds naturally occur in interstellar space.¹



Scheme 1. Crossed Aldol Condensation to synthesize precursor 1-(4-bromophenyl)-3-(4-bromophenyl)prop-2-en-1-one to desired β -diketone product (**1**).

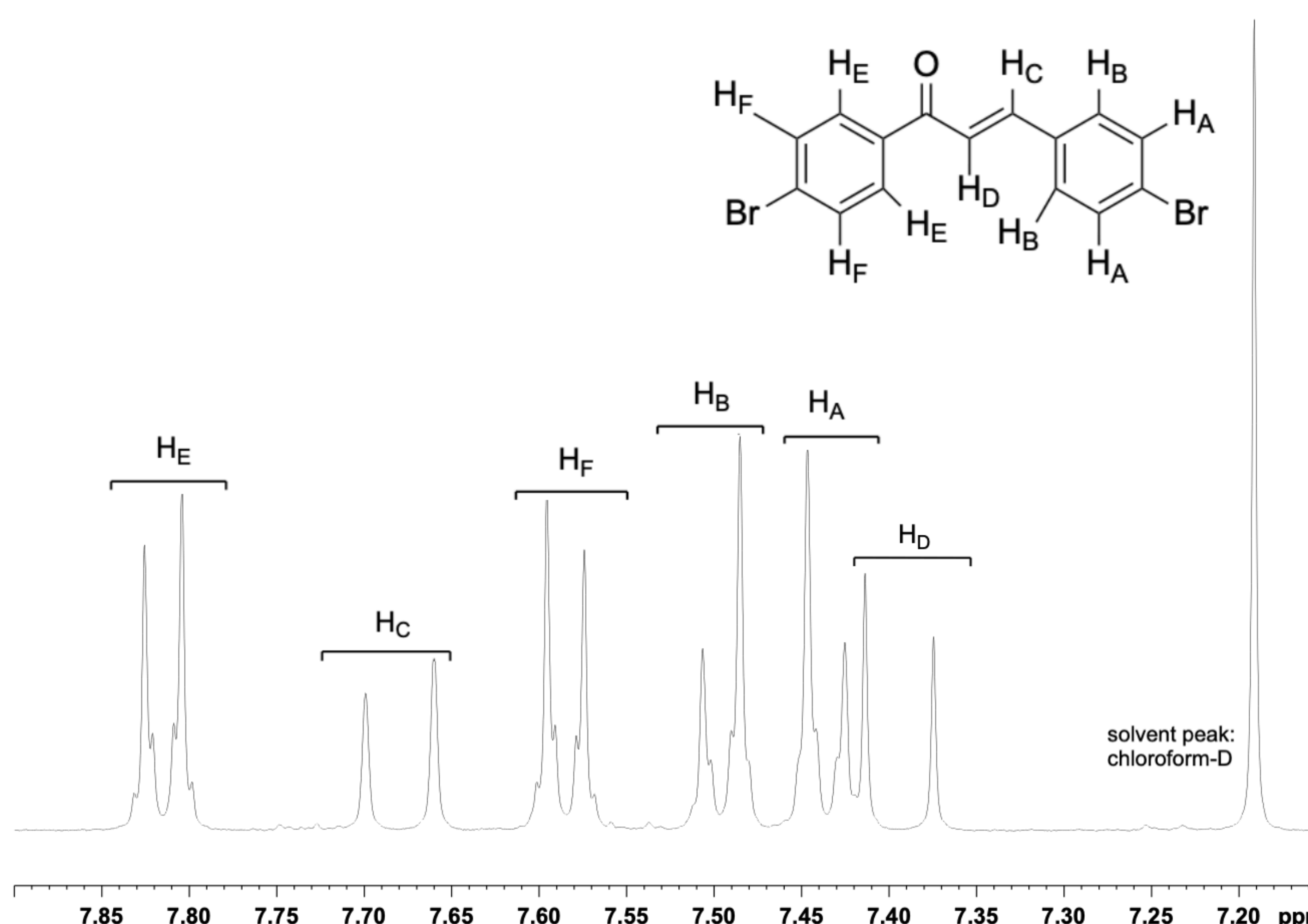
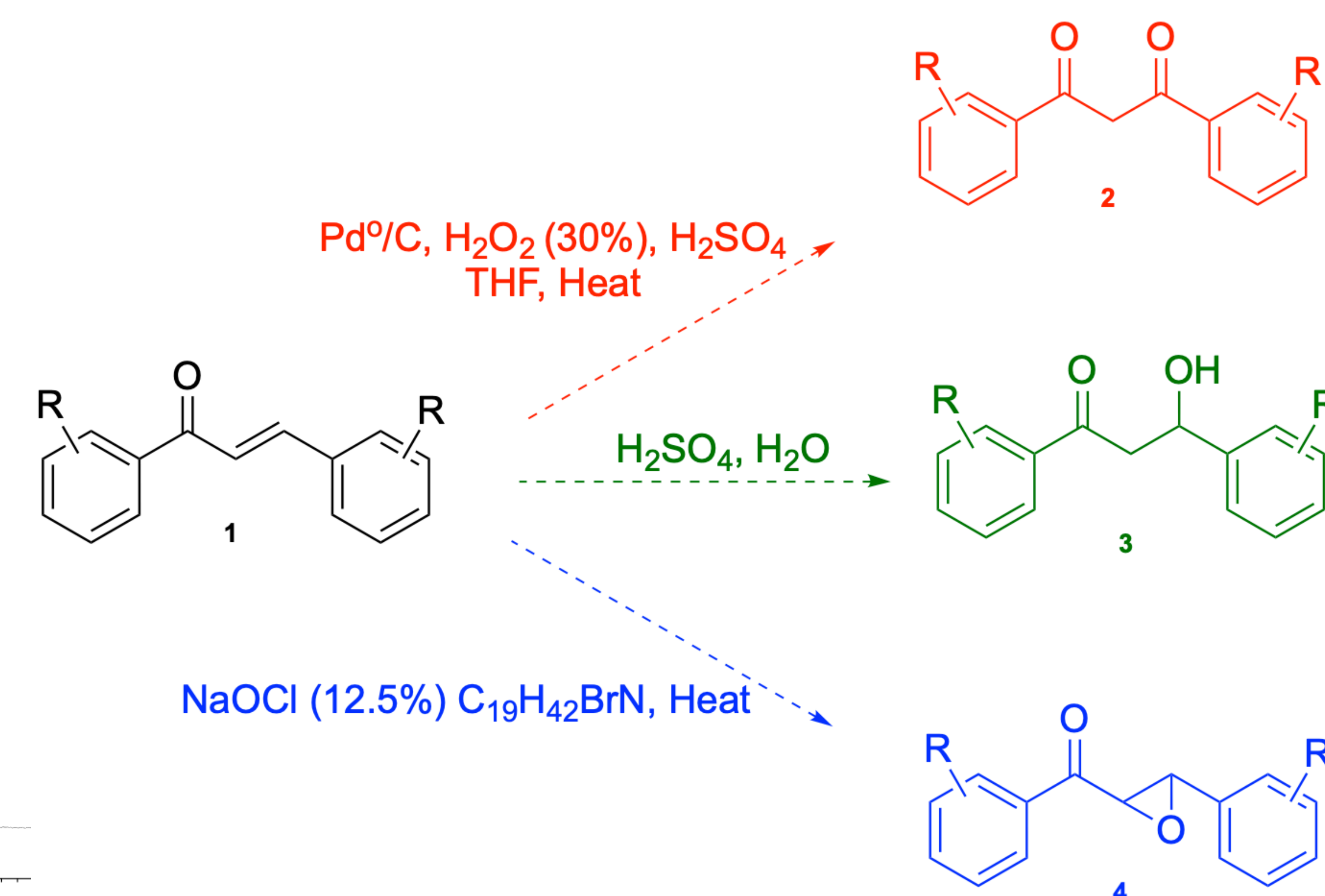


Figure 2. ^1H NMR (400 MHz, CDCl_3) of crossed aldol product, α,β -unsaturated ketone 1-(4-bromophenyl)-3-(4-bromophenyl)prop-2-en-1-one (**1**).



Scheme 2. Proposed oxidation (**2**), hydrolysis (**3**), and epoxidation (**4**) procedures of α,β -unsaturated ketone (**1**).²⁻⁴

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Conclusion:

- Successful synthesis of α,β -unsaturated ketone was accomplished.
- Oxidation, hydrolysis, and epoxidation of α,β -unsaturated ketone (**1**) were unsuccessful.

References:

- (1) <https://earthsky.org/upl/2020/10/dust-interstellar-space-Zeta-Ophiuchi-ripples-e1602268430811.jpg>
- (2) Xiaomeng, X.; Xi, G.; Junhui, X.; Chuanfeng, H.; Xinhua, P. Selective Oxidation of Styrene Derivatives to Ketones over Palladium(0)/Carbon with Hydrogen Peroxide as the Sole Oxidant. *Syn.* **2017**, 28, 5, 607-610. (Accessed 6/10/24).
- (3) Hydration of 1-Hexene. *Montana State University*. **2019**. studocu. Procedure adapted from: <https://www.studocu.com/en-us/document/montana-state-university/elements-of-organic-chemistry/lab-3-hydration-of-1-hexene/7782679> (Accessed 6/17/24).
- (4) Fumio, T. Preparation of Epoxyethylbenzenes. Japan Patent JP11092466, **1999**.