Gas-Phase Synthesis of 3-Vinylcyclopropene via the Crossed Beam Reaction of the Methylidyne Radical (CH; \( \text{X}^2\Pi \)) with 1,3-Butadiene (CH\(_2\)CHCHCH\(_2\); \( \text{X}^1\text{A}_g \))

Chao He, Long Zhao, Srinivas Doddipatla, Aaron M. Thomas, Anatoliy A. Nikolayev, Galiya R. Galimova, Valeriy N. Azyazov, Alexander M. Mebel,* and Ralf I. Kaiser*
Supporting Information

Gas-Phase Synthesis of 3-Vinylcyclopropene via the Crossed Beam Reaction of the Methylidyne Radical (CH; X^2Π) with 1,3-Butadiene (CH\textsubscript{2}CHCH\textsubscript{2}; X\textsuperscript{1A\textsubscript{g}})

Chao He,\textsuperscript{a} Long Zhao,\textsuperscript{a} Srinivas Doddipatla,\textsuperscript{a} Aaron M. Thomas,\textsuperscript{a} Anatoliy A. Nikolayev,\textsuperscript{b} Galiya R. Galimova,\textsuperscript{b,c} Valeriy N. Azyazov,\textsuperscript{b,d} Alexander M. Mebel,\textsuperscript{c,*} Ralf I. Kaiser\textsuperscript{a,*}

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Prof. Alexander M. Mebel: mebela@fiu.edu
Figure S1. Portion of the CsH₇ potential energy surface (PES) leading to p₁-p₆. H atoms from methyldyne radical, CH moiety and CH₂ moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.
Figure S2. Portion of the C₅H₇ PES leading to p7-p11. H atoms from methylidyne radical, CH moiety and CH₂ moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.
Figure S3. Portion of the C₅H₇ PES leading to p1, p5, p6, p9, p12-p14. H atoms from methyldyne radical, CH moiety and CH₂ moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.
Figure S4. Portion of the C₅H₇ PES leading to p1, p2, p6, p11, p15, p16. H atoms from methyldyne radical, CH moiety and CH₂ moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.
Table S1. Rate constants \((k, \text{ in s}^{-1})\) for all unimolecular reactions in the CH + 1,3-butadiene system calculated using RRKM theory at \(E_{\text{col}} = 20.6 \text{ kJ mol}^{-1}\).

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\(k\) constants (in s\(^{-1}\)), \(E_{\text{col}} = 20.6 \text{ kJ mol}^{-1}\).
Optimized Cartesian coordinates (in Å) and calculated vibrational frequencies (in cm\(^{-1}\)) of the reactants, products, intermediates, and transition states in the methyldyne radical plus 1,3-butadiene reaction.

1 INTERMEDIATES

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S16
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Frequencies

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S39
Frequencies

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i13 — p1

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S42
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Frequencies

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Frequencies

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i23 — p13

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S95
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| 1311.3376  | 1439.5257| 1490.8793|
| 1499.2817  | 1572.2530| 1627.7028|
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\[ i36 \rightarrow i37 \]

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|   | 768.2237     | 790.2643     | 916.4957      |               |               |               |               |               |               |               |               |               |               |               |
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i37 — i38

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S111
i17 — i38

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S115
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