Supplementary Information

A Combined Experimental and Theoretical Study on the Formation of the 2-Methyl-1-silacycloprop-2-enylidene Molecule via the Crossed Beam Reactions of the Silylidyne Radical (SiH; $X^2\Pi$) with Methylacetylene (CH_3CCH; X^1A_1) and D4-Methylacetylene (CD_3CCD; X^1A_1)

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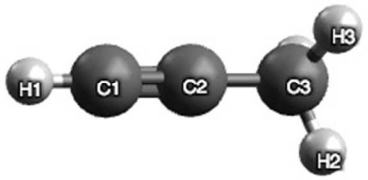
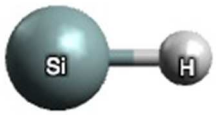
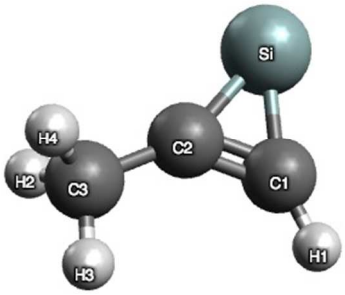
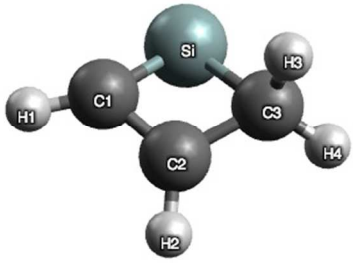
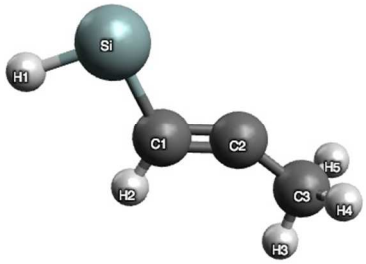
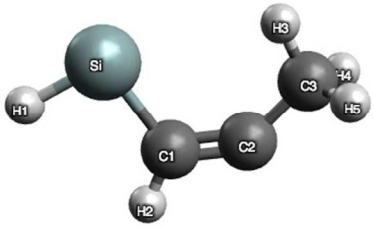
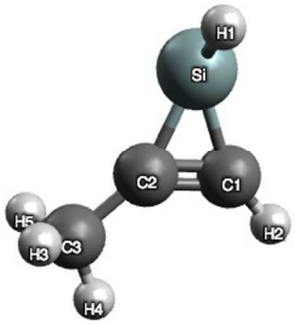
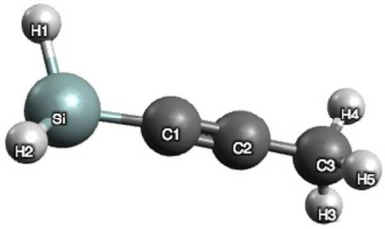
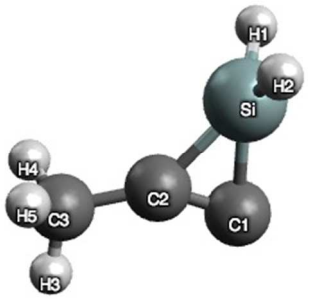
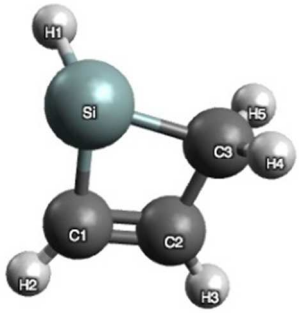
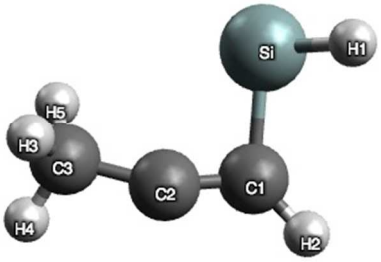
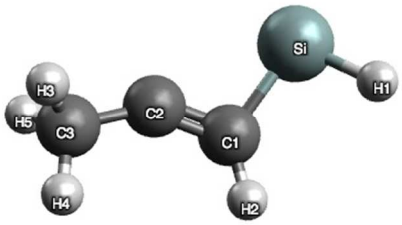
Table S1. Structures of the reactants, products, intermediates, and transition states calculated at the ωB97X-V/cc-pVTZ level of theory. The point groups and symmetries of electronic wave functions are included, with the energies relative to the reactants are given in kJ mol^{-1}. Bond lengths are reported in picometers and angles in degrees. Dark grey: carbon; blue grey: silicon; white: hydrogen.

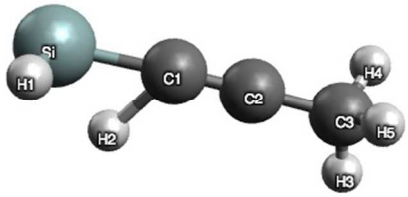
Reactants			
CH_3CCH		SiH	
			
0 $C_{3v} - {}^1A_1$		0 $C_{\infty v} - {}^2\Pi$	
$r(C_1,C_2)$	119.8	r(Si,H)	152.9
$r(C_2,C_3)$	146.3		
$r(C_1,H_1)$	106.5		
$r(C_3,H_2)$	109.2		
$\theta(C_2,C_3,H_2)$	110.6°		
Products			
[p1]		[p2]	
			
-1.01 (CCSD(T)/CBS) $C_s - {}^1A'$		24.0 (CCSD(T)/CBS) $C_1 - {}^1A$	
$r(Si,C_1)$	181.4	$r(Si,C_1)$	183.3
$r(Si,C_2)$	182.7	$r(Si,C_3)$	197.1
$r(C_1,C_2)$	134.3	$r(C_1,C_2)$	136.9
$r(C_2,C_3)$	148.8	$r(C_2,C_3)$	148.4
$r(C_1,H_1)$	1.085	$r(C_1,H_1)$	108.3
$r(C_3,H_2)$	1.094	$r(C_2,H_2)$	109.3
$\theta(Si,C_1,C_2)$	68.9°	$r(C_3,H_3)$	108.7
$\theta(C_1,C_2,C_3)$	137.0°	$\theta(Si,C_1,C_2)$	84.8°
		$\theta(Si,C_3,C_2)$	77.1°
		$\theta(C_1,Si,C_3)$	75.3°
		$\theta(C_1,C_2,C_3)$	109.2°

Intermediates			
[i1]		[i2]	
			
-70.0 $C_s - {}^2A'$		-74.4 $C_s - {}^2A'$	
$r(Si,C_1)$	187.8	$r(Si,C_1)$	188.2
$r(Si,H_1)$	153.1	$r(Si,H_1)$	152.7
$r(C_1,C_2)$	131.6	$r(C_1,C_2)$	131.9
$r(C_2,C_3)$	147.0	$r(C_2,C_3)$	147.0
$r(C_1,H_2)$	109.7	$r(C_1,H_2)$	109.0
$r(C_3,H_3)$	109.8	$r(C_3,H_3)$	109.9
$\theta(Si,C_1,C_2)$	116.8°	$\theta(Si,C_1,C_2)$	118.2°
$\theta(C_1,C_2,C_3)$	142.1°	$\theta(C_1,C_2,C_3)$	139.9°
[i3]		[i4]	
			
-174.1 $C_1 - {}^2A$		-207.6 $C_s - {}^2A'$	
$r(Si,C_1)$	181.2	$r(Si,C_1)$	181.3
$r(Si,C_2)$	182.3	$r(Si,H_1)$	148.6
$r(Si,H_1)$	150.9	$r(C_1,C_2)$	121.0
$r(C_1,C_2)$	134.1	$r(C_2,C_3)$	146.0
$r(C_2,C_3)$	148.7	$\theta(H_1,Si,H_2)$	111.8°
$r(C_1,H_2)$	108.4		
$r(C_3,H_3)$	109.3		
$\theta(Si,C_1,C_2)$	68.8°		
$\theta(C_1,C_2,C_3)$	136.9°		

[i5]		[i6]	
			
-126.6 $C_s - {}^2A'$		-232.4 $C_s - {}^2A'$	
$r(Si,C_1)$	183.1	$r(Si,C_1)$	186.0
$r(Si,C_2)$	189.4	$r(Si,C_3)$	191.5
$r(Si,H_1)$	148.1	$r(Si,H_1)$	150.0
$r(C_1,C_2)$	129.6	$r(C_1,C_2)$	134.5
$r(C_2,C_3)$	148.6	$r(C_2,C_3)$	152.4
$r(C_3,H_3)$	109.2	$r(C_1,H_2)$	108.2
$\theta(Si,C_1,C_2)$	72.3°	$r(C_2,H_3)$	109.1
$\theta(C_1,C_2,C_3)$	149.3°	$r(C_3,H_4)$	109.2
		$\theta(Si,C_1,C_2)$	90.4°

Transition States			
[i1-i2]		[i1-i3]	
			
-66.2 $C_1 - {}^2A$		-68.5 $C_1 - {}^2A$	
$r(Si,C_1)$	188.6	$r(Si,C_1)$	187.3
$r(Si,H_1)$	153.1	$r(Si,H_1)$	153.4
$r(C_1,C_2)$	129.9	$r(C_1,C_2)$	131.2
$r(C_2,C_3)$	146.5	$r(C_2,C_3)$	147.0
$r(C_1,H_2)$	108.9	$r(C_1,H_2)$	109.5
$r(C_3,H_3)$	109.2	$r(C_3,H_3)$	109.3
$\theta(Si,C_1,C_2)$	97.8°	$\theta(Si,C_1,C_2)$	106.1°
$\theta(C_1,C_2,C_3)$	156.1°	$\theta(C_1,C_2,C_3)$	145.3°
$\phi(Si,C_1,C_2,C_3)$	41.8°	$\phi(H_1,Si,C_1,C_2)$	145.2°

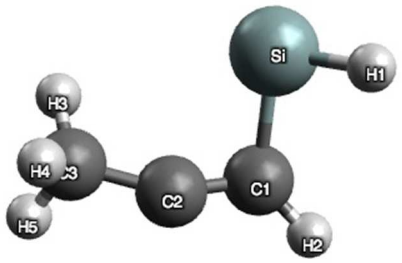
[i1-i4]



-15.1
$C_1 - {}^2A$

$r(Si,C_1)$	185.1
$r(Si,H_1)$	151.6
$r(Si,H_2)$	163.9
$r(C_1,C_2)$	124.0
$r(C_2,C_3)$	145.5
$r(C_1,H_2)$	151.7
$r(C_3,H_3)$	109.5
$\theta(Si,C_1,C_2)$	171.6°

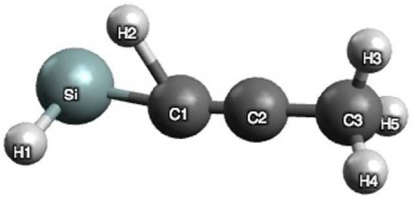
[i2-i3]



-66.1
$C_1 - {}^2A$

$r(Si,C_1)$	188.6
$r(Si,H_1)$	153.0
$r(C_1,C_2)$	130.0
$r(C_2,C_3)$	146.5
$r(C_1,H_2)$	108.9
$r(C_3,H_3)$	109.7
$\theta(Si,C_1,C_2)$	97.8°
$\theta(C_1,C_2,C_3)$	155.8°
$\phi(H_1,Si,C_1,C_2)$	126.8°

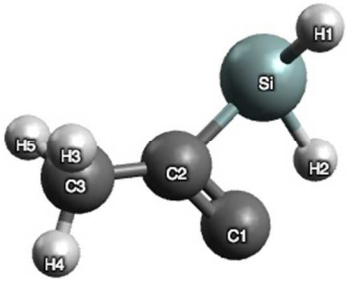
[i2-i4]



-15.1
$C_1 - {}^2A$

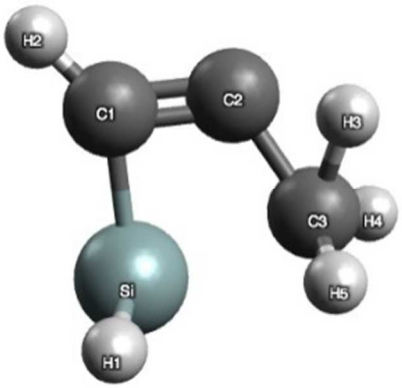
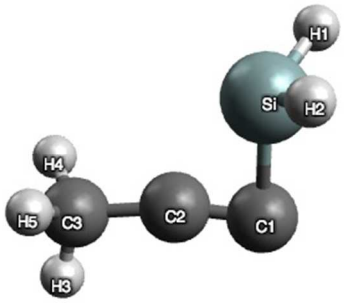
$r(Si,C_1)$	185.1
$r(Si,H_1)$	151.6
$r(Si,H_2)$	163.9
$r(C_1,C_2)$	124.0
$r(C_2,C_3)$	145.5
$r(C_1,H_2)$	151.7
$r(C_3,H_3)$	109.5
$\theta(Si,C_1,C_2)$	171.4°

[i3-i5]



2.8
$C_1 - {}^2A$

$r(Si,C_1)$	218.2
$r(Si,C_2)$	182.0
$r(Si,H_1)$	150.1
$r(Si,H_2)$	155.2
$r(C_1,C_2)$	132.5
$r(C_2,C_3)$	149.5
$r(C_1,H_2)$	160.3
$r(C_3,H_3)$	109.2
$\theta(Si,C_2,C_1)$	86.3°
$\theta(C_1,C_2,C_3)$	132.2°

[i3-i6]		[i4-i5]	
			
136.3 $C_1 - {}^2A$		-114.1 $C_s - {}^2A'$	
r(Si,C_1)	190.5	r(Si,C_1)	186.4
r(Si,C_2)	230.0	r(Si,C_2)	217.7
r(Si,C_3)	212.6	r(Si,H_1)	148.5
r(Si,H_1)	153.3	r(C_1,C_2)	124.8
r(C_1,C_2)	131.9	r(C_2,C_3)	146.8
r(C_2,C_3)	155.0	r(C_3,H_3)	109.3
r(C_1,H_2)	108.1	θ(Si,C_1,C_2)	86.4°
r(C_2,H_3)	131.9	θ(C_1,C_2,C_3)	169.3°
r(C_3,H_3)	126.1		
r(C_3,H_4)	108.2		
θ(Si,C_1,C_2)	89.1°		
θ(Si,C_3,C_2)	75.7°		
θ(C_1,Si,C_3)	75.3°		