Supporting Information of

Elucidating the toluene formation mechanism in the reaction of propargyl radical with 1,3-butadiene

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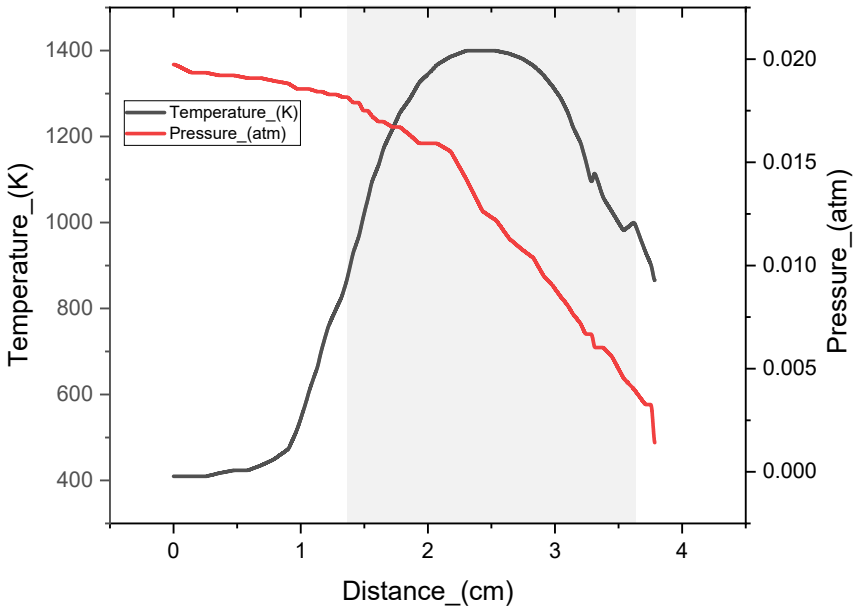

Figure S1. The temperature and pressure profiles within the reactor used in the SiC reaction simulation. The grey shaded area defines the heated section of the SiC tube. The line shapes are taken from ref. [4].

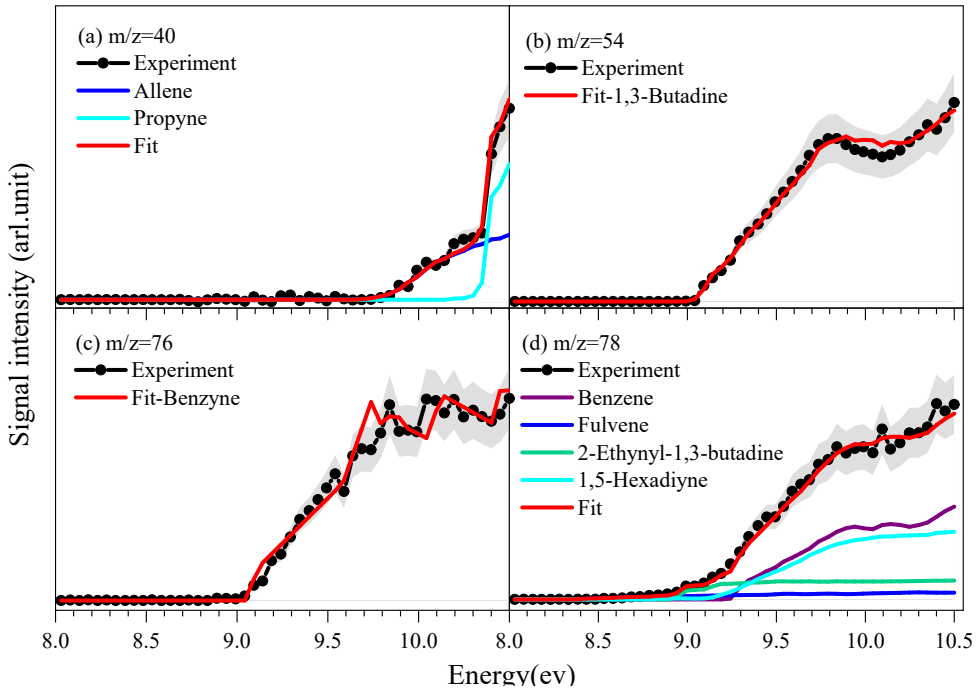

Figure S2. Photoionization efficiency (PIE) curves for signal at m/z = 39 (a) [1], 54 (b) [2], 76 (c) [3], and (d) 78 [4] in the propargyl addition to 1,3-butadiene reactions at the temperature of 1400 K. Black dots: experimentally derived PIE curves; colored lines (green, blue, purple): reference PIE curves; red line: overall fit; The overall error shades are ± 15% signal intensity based on the accuracy of the photodiode.

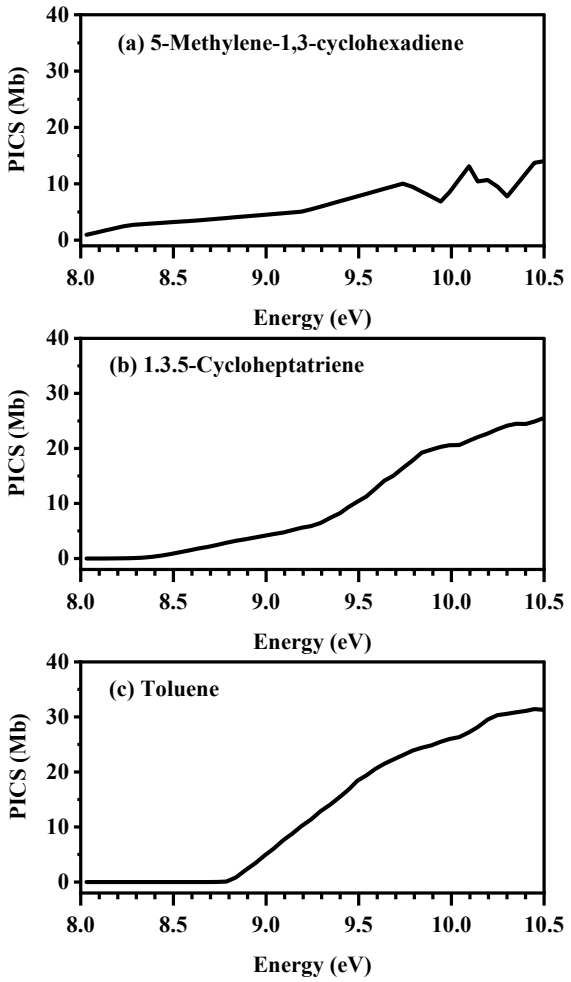

Figure S3. Absolute photoionization cross sections (PICS) of 5-methylene-1,3-cyclohexadiene (a), 1,3,5-cycloheptatriene (b), and toluene (c). (a)-(c) are taken from the references [3, 5], and (b) is measured in this work. (a) is the estimated PICS.

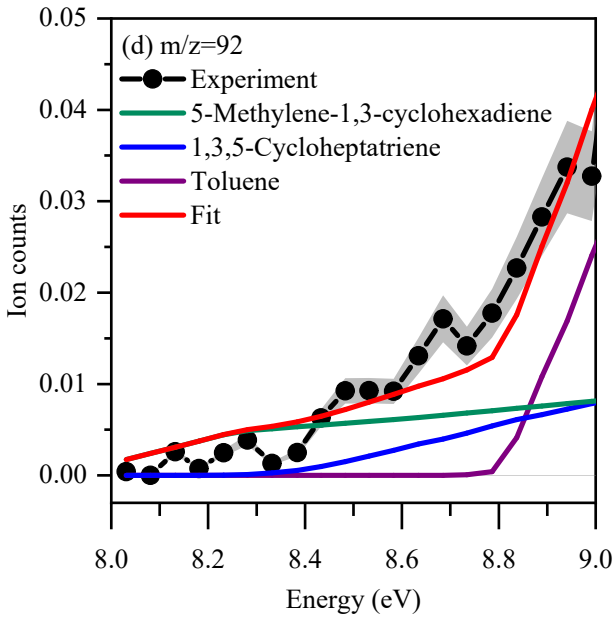

Figure S4. Photoionization efficiency (PIE) curve in the energy of 8-9 eV for the signal at m/z = 92 in the propargyl addition to 1,3-butadiene reactions at the temperature of 1400 K. Black and dotted curve: experimentally derived PIE curves; colored lines: reference PIE curves; and red lines: overall fit.

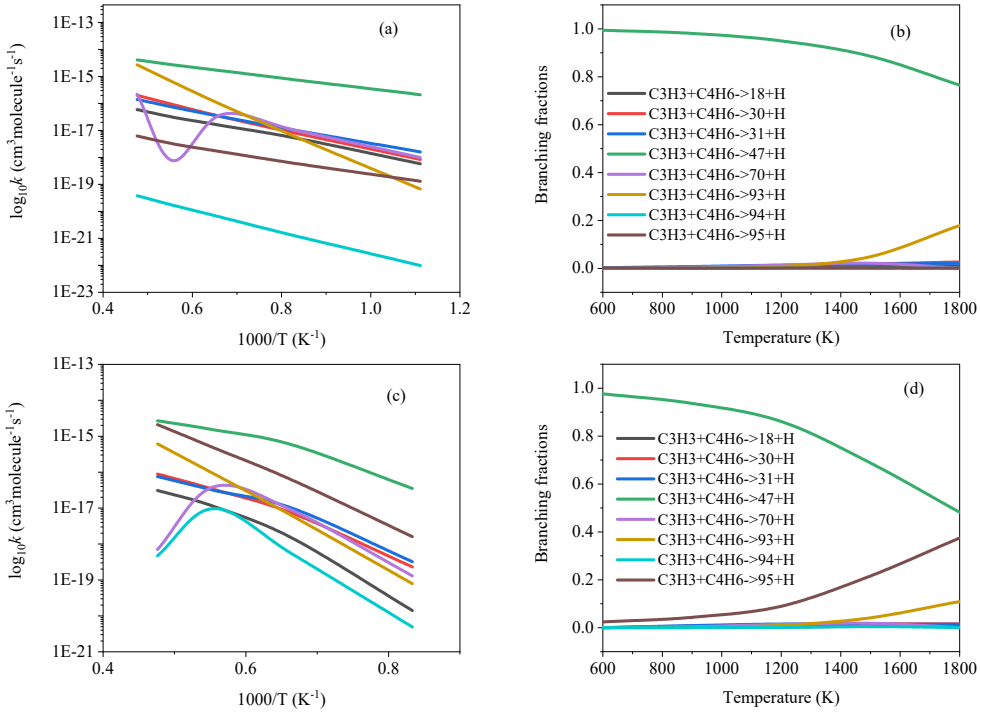

Figure S5. Calculated rate coefficients and the corresponding branching fractions for the propargyl addition to 1,3-butadiene leading to different C_7H_8 isomeric products at 7.6 Torr (a)-(b), at 760 Torr (c)-(d) at the CBS-QB3 level [6].

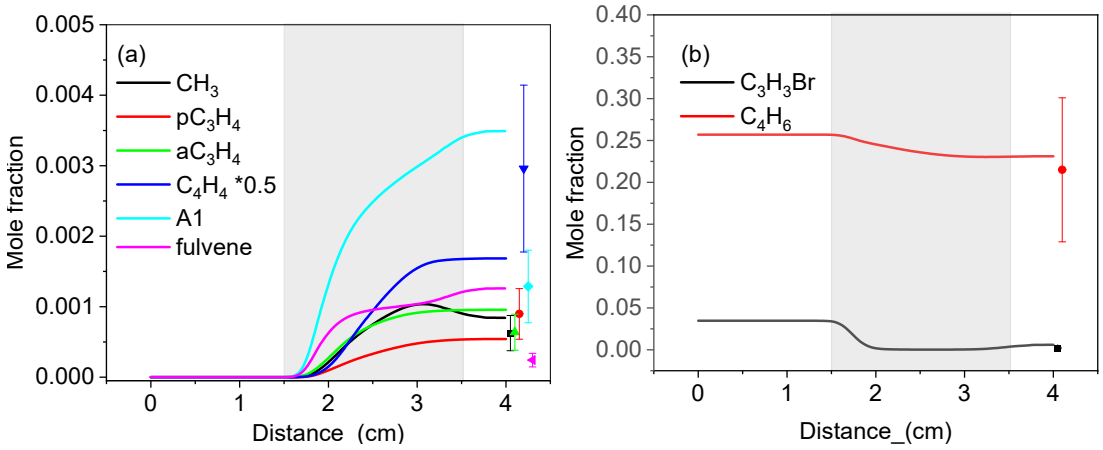

Figure S6. Simulated profiles (lines) and experimental measurements (open symbols with the error bars) of the mole fraction ratios of C_3H_4, C_4H_4, C_3H_3Br, C_4H_6 along the reactor axis. The experimental measurements are presented at different x positions for clarity. The grey shaded area defines the heated section of the SiC tube.

Table S1. Relative enthalpies (ΔH), and Gibbs free energies (ΔG) of isomerization reactions from 47 to 101, and 47 to 44 calculated at different levels of theory. Units are in kcal/mol. For the CCSD(T), the structures are optimized at the level of M06-2X/6-311+G(d, p).

	M06-2X/6-311+G(d, p)		CCSD(T)/6-311+G(d, p)		CCSD(T)/CBS	
	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
47	0	0	0	0	0	0
TS47-101	75.0	75.5	77.7	78.2	77.5	78.0
101	71.6	71.5	70.4	70.3	72.0	71.9
TS47-44	60.4	60.8	64.4	64.7	61.4	61.7
44	-33.5	-34.2	-30.6	-31.3	-31.7	-32.4

Table S2. Calculated rate constants for H-assisted isomerization and unimolecular isomerization between 5-methylene-1,3-cyclohexadiene 47, toluene 44, and 1,3,5-cycloheptatriene 9 at the pressure of 7.6, 22.8, 76, 760 torr, respectively.

□	H-assisted ($cm^3mol^{-1}s^{-1}$)				□	Unimolecular (s^{-1})		
T/reaction	47+H→9+H	9+H→47+H	47+H→44+H	44+H→47+H	47→9	9→47	47→44	44→47
600	5.32E+04	1.64E+05	1.58E+13	7.48E+00	1.28E-16	3.91E-16	5.16E-11	3.07E-22
800	6.15E+06	2.06E+07	3.15E+13	8.53E+03	1.66E-09	5.43E-09	3.78E-05	1.65E-13
1000	9.99E+07	3.53E+08	5.14E+13	6.34E+05	2.76E-05	9.36E-05	1.33E-01	3.13E-08
1200	6.68E+08	2.46E+09	7.49E+13	1.19E+07	1.32E-02	4.53E-02	2.72E+01	9.36E-05
1400	2.77E+09	1.06E+10	1.01E+14	1.00E+08	6.93E-01	2.38E+00	8.94E+02	2.12E-02
1600	8.38E+09	3.27E+10	1.29E+14	5.10E+08	8.67E+00	2.96E+01	8.39E+03	8.55E-01
1800	2.01E+10	8.01E+10	1.58E+14	1.83E+09	4.47E+01	1.54E+02	3.53E+04	1.13E+01
2000	4.07E+10	1.64E+11	1.86E+14	5.12E+09	1.44E+02	5.12E+02	9.31E+04	7.45E+01

P=7.6torr

□	H-assisted ($cm^3mol^{-1}s^{-1}$)				Unimolecular (s^{-1})			
T/reaction	47+H→9+H	9+H→47+H	47+H→44+H	44+H→47+H	47→9	9→47	47→44	44→47
600	2.49E+04	7.66E+04	1.57E+13	7.44E+00	1.28E-16	3.91E-16	5.16E-11	3.07E-22
800	4.45E+06	1.48E+07	3.15E+13	8.53E+03	1.68E-09	5.50E-09	3.78E-05	1.65E-13
1000	9.14E+07	3.23E+08	5.14E+13	6.34E+05	3.00E-05	1.02E-04	1.35E-01	3.19E-08
1200	6.55E+08	2.42E+09	7.49E+13	1.19E+07	1.70E-02	5.83E-02	3.03E+01	1.04E-04
1400	2.77E+09	1.05E+10	1.01E+14	1.00E+08	1.11E+00	3.82E+00	1.17E+03	2.77E-02
1600	8.38E+09	3.27E+10	1.29E+14	5.10E+08	1.72E+01	5.87E+01	1.32E+04	1.34E+00
1800	2.01E+10	8.01E+10	1.58E+14	1.83E+09	1.04E+02	3.53E+02	6.41E+04	2.04E+01
2000	4.07E+10	1.64E+11	1.86E+14	5.12E+09	3.59E+02	1.24E+03	1.86E+05	1.49E+02

P=22.8Torr

□	H-assisted ($cm^3mol^{-1}s^{-1}$)				Unimolecular (s^{-1})			
T/reaction	47+H→9+H	9+H→47+H	47+H→44+H	44+H→47+H	47→9	9→47	47→44	44→47
600	9.06E+03	2.79E+04	1.51E+13	7.14E+00	1.28E-16	3.92E-16	5.16E-11	3.07E-22
800	2.52E+06	8.40E+06	3.14E+13	8.50E+03	1.69E-09	5.52E-09	3.79E-05	1.65E-13
1000	7.35E+07	2.60E+08	5.14E+13	6.34E+05	3.12E-05	1.06E-04	1.37E-01	3.22E-08
1200	6.14E+08	2.26E+09	7.49E+13	1.19E+07	2.00E-02	6.86E-02	3.23E+01	1.11E-04
1400	2.76E+09	1.05E+10	1.01E+14	1.00E+08	1.62E+00	5.55E+00	1.43E+03	3.39E-02
1600	8.36E+09	3.26E+10	1.29E+14	5.10E+08	3.15E+01	1.07E+02	1.93E+04	1.97E+00
1800	2.01E+10	8.00E+10	1.58E+14	1.83E+09	2.31E+02	7.80E+02	1.12E+05	3.57E+01
2000	4.07E+10	1.64E+11	1.86E+14	5.12E+09	9.04E+02	3.06E+03	3.68E+05	2.95E+02

P=76Torr

□	H-assisted ($cm^3mol^{-1}s^{-1}$)			□	Unimolecular (s^{-1})			□
T/reaction	47+H→9+H	9+H→47+H	47+H→44+H	44+H→47+H	47→9	9→47	47→44	44→47
600	9.02E+02	2.78E+03	8.66E+12	4.09E+00	1.28E-16	3.92E-16	5.16E-11	3.07E-22
800	4.44E+05	1.48E+06	2.76E+13	7.47E+03	1.69E-09	5.53E-09	3.79E-05	1.65E-13
1000	2.64E+07	9.33E+07	5.03E+13	6.21E+05	3.17E-05	1.08E-04	1.37E-01	3.24E-08
1200	3.79E+08	1.40E+09	7.47E+13	1.18E+07	2.21E-02	7.58E-02	3.35E+01	1.15E-04
1400	2.21E+09	8.41E+09	1.01E+14	1.00E+08	2.24E+00	7.70E+00	1.68E+03	4.00E-02
1600	7.66E+09	2.99E+10	1.29E+14	5.10E+08	6.32E+01	2.15E+02	2.95E+04	3.01E+00
1800	2.00E+10	7.95E+10	1.58E+14	1.83E+09	6.90E+02	2.32E+03	2.35E+05	7.49E+01
2000	4.06E+10	1.64E+11	1.86E+14	5.12E+09	3.74E+03	1.24E+04	1.03E+06	8.21E+02

P=760Torr

Table S3. Kinetic parameters for reactions updated in the SiC model.

□	reaction	A	n	Ea(cal)	Factor	Ref.
R12	1,3-C_4H_6=C_2H_4+C_2H_2	6.40E+13	0.00	77100	×1	[7][b]
R13	1,3-C_4H_6=1,2-C_4H_6	8.19E+74	-17.56	115782	×1	[8][b]
R14	C_3H_3+CH_3 (+M)=1,2-C_4H_6 (+M)	□			×1	[9][b]
□	k_0	2.60E+58	-11.94	9770		
□	k_∞	1.50E+13	0.00	0		
□	F_{cent}[e]	0.175(α)	1.34E+3(T***)	6.00E+4(T*)	9.77E+3(T**)	
R15	1,3-C_4H_6+Br=HBr+*i*-C_4H_5	3.01E+10	0.00	0	×1	[10][b]
R16	C_4H_4+H = *i*-C_4H_5	□	□	□	×1	[11][b]
□	0.013atm	6.10E+53	-13.19	14200		
□	0.026atm	9.60E+52	-12.85	14300		
□	0.118atm	2.10E+52	-12.44	15500		
□	1atm	4.90E+51	-11.92	17700		
□	10atm	1.50E+48	-10.58	18800		
R23	C_3H_3+C_4H_4=$C_6H_5CH_2$				×1	[12][c]
	0.1atm	6.84E+82	-20.80	60200		
R18	1,3-C_4H_6 + C_3H_3 =C_7H_8 (47) + H				×2	[13][c]
	0.1atm	1.80E+07	0.86	6887		
R9	C_3H_3Br = C_3H_3+Br	4.52E+12	-0.52	36983		[4][b]
R6(a)	1,3-C_4H_6+C_3H_3 =1,3-NC_4H_5+a-C_3H_4	1.00E+13	0.00	22500		[7][b]
R6(b)	1,2-C_4H_6+C_3H_3 =1,2-C_4H_5+a-C_3H_4	5.00E+12	0.00	19522		[7][b]
R7	C_3H_3+C_3H_3=C_6H_5+H	□	□	□	×0.1	[14][b]
□	0.03947atm	1.05E+54	-11.88	28757		
□	1atm	1.70E+48	-9.98	36755		
□	10atm	3.67E+26	-3.88	28963		
R10(a)	C_3H_3+C_3H_3=fulvene	□	□	□	×0.1	[14][b]
□	0.03947atm	6.30E+76	-19.07	31542		
□	1atm	1.38E+66	-15.66	28260		
□	10atm	1.26E+56	-12.61	23515		
R10(b)	C_3H_3+C_3H_3=A1 (benzene)	□	□	□	×0.1	[14][b]
□	0.03947atm	1.82E+74	-18.14	31896		
□	1atm	3.16E+55	-12.55	22264	/	
□	10atm	3.89E+50	-11.01	20320		
R17	$C_6H_5CH_3$ (+M) =C_6H_5+CH_3 (+M)	□	□	□	×1	[15][b]
□	k_0	1.00E+98	-22.97	122080		
□	k_∞	1.95E+27	-3.16	107447		
□	F_{cent}[e]	0.705(α)	1.00E+10(T***)	4.60E+2(T*)	8.21E+9(T**)	

Table S3. Continued table.

R11	$C_6H_5CH_2+H=C_6H_5+CH_3$	□	□	□	×1	□[16][b]
□	0.0395	4.50E+58	-11.9	51860		□
□	0.132	2.03E+64	-13.37	59520		□
□	1	5.83E+67	-14.15	68330		□
□	10	8.85E+68	-14.23	78410		□
R8(a)	C_6H_5 (+M)=o-C_6H_4+H (+M)	□	□	□	×1	□[17][b]
□	k_0	1.00E+84	-18.87	90064		□
□	k_∞	4.30E+12	0.62	77313		□
□	F_{cent}[e]	0.902(α)	696(T***)	358(T*)	3856(T**)	□
R8(b)	C_6H_5 + C_6H_5 =A1+o-C_6H_4	1.71E-03	4.57	-5739		□[18][b]
R2	$C_6H_5CH_3$ (+M) =$C_6H_5CH_2$+H (+M)	□	□	□	×1	□[15][b]
□	k_0	1.00E+98	-22.86	99882		□
□	k_∞	2.78E+15	0.17	91168		□
□	F_{cent}[e]	0.065(α)	15.11(T***)	1.00E+10(T*)	7.60E+7(T**)	□
R19	C_7H_8 (47) =$C_6H_5CH_3$ (44)	□	□	□	×1	This work
□	0.01atm	1.57E+49	-10.92	76070.0947		□
□	0.03atm	2.05E+44	-9.41	73984.3664		□
□	0.10atm	9.08E+38	-7.76	72261.3277		□
R20	C_7H_8 (47) + H = $C_6H_5CH_3$ (44) +H	□	□	□	×1	This work
□	0.01atm	6.81E+10	1.11	2030		□
□	0.03atm	7.13E+10	1.10	2040		□
□	0.1atm	9.69E+10	1.07	2150		□
R21	C_3H_3+*i*-C_4H_5= $C_6H_5CH_3$ (44)	□	□	□	×0.1	□[14][d]
□	0.03947atm	1.82E+74	-18.14	31896		□
□	1atm	3.16E+55	-12.55	22264		□
□	10atm	3.89E+50	-11.01	20320		□
R22	C_3H_3+*i*-C_4H_5=$C_6H_5CH_2$+H	□	□	□	×0.1	□[14][d]
□	0.03947atm	1.05E+54	-11.88	28757		□
□	1atm	1.70E+48	-9.98	36755		□
□	10atm	3.67E+26	-3.88	28963		□

[a] Rate conslants are given in the form, $k = AT^n exp(-Ea/RT)$. The units are cm^3,Mol,cal, s, and K

[b] Take from literature

[c] Rate constant estimated from the value given in reference.

[d] Estimated by analogy with the $C_3H_3+C_3H_3$ reactions of literature[14].

[e] $Fcent=(1-\alpha)exp(-T/T***)+\alpha exp(-T/T*)+exp(-T**/T)$

Table S4. The simulated and experimental mole fractions of all species at the exit of the microreactor.

□	X_i (Model)	$X_i^a \pm \Delta X_i^b$ (Exp.)
C_3H_3Br	5.98E-03	(2.15±0.86)E-3
$C_6H_6CH_2$ (47)	1.43E-04	(1.93±0.77)E-4
C_7H_8 (9)	1.00E-07	(1.20±0.48)E-4
CH_3	8.42E-04	(6.25±2.50)E-4
C_3H_3	8.91E-03	(4.89±1.96)E-3
pC_3H_4	5.41E-04	(8.98±3.59)E-4
aC_3H_4	9.56E-04	(6.38±2.55)E-4
C_4H_4	3.37E-03	(5.92±2.37)E-3
C_4H_6	2.31E-01	(2.12±0.85)E-1
A1	3.49E-03	(1.29±0.52)E-3
fulvene	1.26E-03	(2.42±0.97)E-4
$A1CH_3$ (44)	3.98E-04	(3.01±1.20)E-4
$C_6H_5CH_2$	2.20E-04	(3.62±1.45)E-4

[a] Mole fraction calculated by $X_i(T) = X_A(T)\frac{S_i(T,E)\,\sigma_A(E)D_A}{S_A(T,E)\,\sigma_i(E)\,D_i}$, where T and E is selected at 1400 K, 10.5 eV, respectively. S is the integral intensity of the mass spectral signal, and σ is the photoionization cross-section, and D is the mass discrimination factor.

[b] The estimated error consists of ΔS (15%) + $\Delta\sigma$ (15%) + ΔD (10%).

Table S5. CCSD(T)//M06-2X geometries, energies, and vibrational frequencies.

9

Atom	X	Y	Z	(Angstrom)
C	0.9629	-1.22165	-0.2019	
C	1.46122	0	0.52803	
C	0.9629	1.22165	-0.2019	
C	-0.34762	1.52755	-0.26608	
C	-1.42868	0.68081	0.18605	
C	-1.42868	-0.68081	0.18605	
C	-0.34762	-1.52755	-0.26608	
H	1.68919	-1.87563	-0.67539	
H	2.55047	0	0.59061	
H	1.06693	0	1.5529	
H	-2.36558	-1.17803	0.42349	
H	1.68919	1.87563	-0.67539	
H	-0.63557	2.47637	-0.71232	
H	-2.36558	1.17803	0.42349	
H	-0.63557	-2.47637	-0.71232	

ZPE	**0.128984**	(Hartree)
CCSD(T)/cc-pVDZ	**-270.82747**	(Hartree)

Frequencies cm^{-1}:

235.4635	293.7084	359.4857	411.8169	433.2483	613.416
668.3199	735.9959	770.1913	820.8595	887.0635	938.5021
953.7725	978.9767	999.5364	1005.6678	1022.5305	1048.3037
1075.3998	1207.3421	1222.0572	1246.8535	1271.8856	1329.9344
1383.762	1423.212	1480.267	1482.0079	1618.726	1701.6741
1703.6296	3039.8262	3140.14	3166.7047	3175.05	3179.0527
3190.8563	3199.2646	3202.9016			

44

Atom	X	Y	Z	(Angstrom)
C	0.19274	1.20064	-0.00818	
C	-1.20056	1.20198	0.00205	
C	-1.90155	-0.00127	0.00793	
C	-1.19736	-1.20371	0.00184	
C	0.19494	-1.19937	-0.00836	
C	0.91234	0.00191	-0.01101	
H	-1.73786	2.14408	0.00169	
H	-2.98568	-0.00267	0.01304	
H	-1.73292	-2.14682	0.00126	
H	0.73386	-2.1418	-0.0167	

C	2.42193	0.00076	0.00882
H	2.82717	0.93345	-0.39003
H	2.80237	-0.11177	1.03017
H	2.82864	-0.82417	-0.58161
H	0.72951	2.14415	-0.01638

ZPE **0.128586** (Hartree)
CCSD(T)/cc-pVDZ **-270.8761935** (Hartree)

Frequencies cm^{-1}：

33.8284	210.5402	346.1739	412.3978	474.5556	528.4594
633.9038	713.8824	750.1268	806.3541	867.8624	926.0072
999.9699	1005.6584	1018.417	1019.4814	1062.7311	1066.9178
1117.3985	1177.8431	1204.4971	1244.9023	1322.4747	1352.7428
1416.7006	1476.5431	1495.4939	1510.3399	1541.4403	1658.7386
1681.1605	3062.1688	3125.2667	3147.9584	3190.5136	3192.473
3205.7772	3214.7347	3226.2724			

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Atom	X	Y	Z	(Angstrom)
C	-0.24022	-1.27891	0.17521	
C	1.23895	-1.14408	-0.07881	
C	1.83995	0.0514	-0.11526	
C	1.06857	1.28183	0.03626	
C	-0.27745	1.26153	0.09869	
C	-1.03287	0.01414	0.02484	
C	-2.36356	0.01298	-0.15152	
H	1.8139	-2.05834	-0.18514	
H	-0.66743	-2.05931	-0.4626	
H	-0.36715	-1.64814	1.20535	
H	1.60008	2.22694	0.06172	
H	2.91205	0.12548	-0.26243	
H	-0.84005	2.18803	0.15547	
H	-2.92817	-0.90817	-0.24509	
H	-2.92345	0.94013	-0.20381	

ZPE **0.127793** (Hartree)
CCSD(T)/cc-pVDZ **-270.8264475** (Hartree)

Frequencies cm^{-1}：

92.5384	261.3544	381.8713	429.794	476.5927	555.7617
593.1671	671.0025	756.171	779.1488	827.4267	916.8121
938.0984	952.3805	967.7736	985.5641	1007.8918	1011.8624
1032.5444	1178.0697	1200.8445	1223.7233	1315.5304	1345.2604
1399.4621	1436.1939	1451.1561	1469.6255	1657.12	1701.162
1739.4503	3005.8559	3101.8283	3162.5363	3190.2176	3195.4045
3211.166	3221.6491	3250.5169			

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Atom	X	Y	Z	(Angstrom)
C	−0.2527	−1.20946	0.34118	
C	1.83461	0.14109	−0.02812	
C	1.09125	1.28611	0.08342	
C	−0.31834	1.269	0.01611	
C	−1.05404	0.04527	0.03094	
C	−2.39891	0.00227	−0.15402	
H	−0.79521	−2.0997	0.01423	
H	−0.15427	−1.27788	1.43248	
H	1.59601	2.24256	0.17999	
H	2.91809	0.18604	−0.01795	
H	−0.86392	2.2044	−0.05031	
H	−2.94574	−0.93325	−0.13323	
H	−2.97153	0.90678	−0.32732	
C	1.15861	−1.17966	−0.26901	
H	1.09686	−1.35408	−1.35474	
H	1.75681	−2.00255	0.13385	

ZPE **0.137936** (Hartree)

CCSD(T)/cc-pVDZ **-271.4117074** (Hartree)

Frequencies cm^{-1}：

139.4743	215.8841	367.551	393.8965	493.2061	501.4165
560.2986	644.5814	688.1269	752.9444	791.8461	809.9272
890.2891	907.1805	961.6352	976.021	989.9147	1033.581
1052.28	1095.7953	1169.297	1186.9307	1226.0874	1310.5723
1330.734	1356.8293	1376.0067	1436.3022	1442.8414	1473.0904
1483.8147	1554.8841	1613.8418	3014.463	3048.2505	3103.193
3119.2685	3166.5917	3190.1516	3203.218	3215.0826	3259.4637

113

Atom	X	Y	Z	(Angstrom)
C	−1.36223	0.62796	−0.42099	
C	−1.52537	−0.81082	0.12444	
C	−0.26917	−1.5754	0.12113	
C	1.02846	−1.36513	−0.00185	
C	1.69233	−0.0541	−0.11846	
C	1.13806	1.15975	0.01148	
H	−2.33546	1.12443	−0.3437	
H	−2.27544	−1.33316	−0.48315	
H	−1.93522	−0.78314	1.14207	
H	1.79629	2.01797	−0.09436	
H	−1.11327	0.57958	−1.48503	
H	1.69477	−2.22753	−0.00901	
H	2.76036	−0.10132	−0.3157	

C	−0.30756	1.48105	0.30821
H	−0.47776	1.41232	1.39231
H	−0.48139	2.53105	0.05282

ZPE **0.139296** (Hartree)
CCSD(T)/cc-pVDZ **-271.3628697** (Hartree)

Frequencies cm^{-1}：

95.1778	234.0644	332.264	365.4911	381.2489	498.7873
580.2818	714.3683	781.3163	803.0573	846.0144	879.5674
885.0462	926.5293	964.0845	1008.718	1049.8052	1067.3611
1089.5065	1179.8729	1230.4613	1253.477	1281.0317	1310.0338
1359.0455	1367.2037	1370.5852	1427.3171	1469.1101	1481.7535
1491.1073	1703.0885	1750.1809	3034.285	3049.2051	3067.1771
3081.9095	3110.8507	3117.3874	3139.6593	3172.2905	3194.0589

114

Atom	X	Y	Z	(Angstrom)
C	−0.10409	−0.06143	−0.01672	
C	−0.08444	−0.0422	1.50544	
C	1.24366	0.13724	2.22646	
C	2.46478	0.20989	1.41004	
C	2.42644	−0.034	0.04109	
C	1.24655	−0.22376	−0.6538	
C	0.4779	−1.18964	2.28864	
H	1.27588	−0.41863	−1.72042	
H	3.40848	0.41027	1.90441	
H	0.91017	−2.02015	1.74235	
H	0.00626	−1.4536	3.22815	
H	−0.93344	0.46124	1.95659	
H	−0.78549	−0.84787	−0.37073	
H	−0.54716	0.88102	−0.37263	
H	1.24007	0.72093	3.14087	
H	3.36332	−0.06998	−0.50723	

ZPE **0.138894** (Hartree)
CCSD(T)/cc-pVDZ **-271.3921887** (Hartree)

Frequencies cm^{-1}：

153.9231	286.8998	349.1289	488.3062	516.7254	571.2776
634.8693	726.5443	763.1714	824.5694	837.9647	866.8271
916.4142	949.9365	973.6427	1011.0563	1019.6855	1041.2243
1072.0875	1113.8682	1119.5472	1152.3261	1167.7567	1224.4494
1241.8834	1341.0869	1354.0826	1405.8608	1422.388	1441.3395
1474.0442	1501.9447	1534.6119	3019.6578	3050.4107	3155.5425
3182.26	3188.1952	3194.1112	3205.9933	3220.2441	3251.6536

115

Atom	X	Y	Z	(Angstrom)
C	-0.12001	-0.29255	-0.1137	
C	0.17897	0.0327	1.28052	
C	1.3892	0.14017	1.84845	
C	2.69141	-0.08031	1.1039	
C	2.69265	-1.40782	0.41113	
C	1.98775	-1.57494	-0.89078	
C	0.6296	-0.927	-1.03132	
H	-1.10685	0.02565	-0.44324	
H	-0.68921	0.24857	1.89819	
H	2.81157	0.72385	0.36295	
H	1.45094	0.38982	2.90395	
H	3.53134	-0.00212	1.79926	
H	3.0425	-2.28134	0.94814	
H	1.87903	-2.64329	-1.12016	
H	2.61202	-1.18334	-1.71679	
H	0.19702	-1.03559	-2.02418	

ZPE **0.137599** (Hartree)

CCSD(T)/cc-pVDZ **-271.3768847** (Hartree)

Frequencies cm-1：

89.7537	186.3417	307.9155	328.0935	382.0368	401.6038
523.5715	633.0943	705.1583	790.8626	845.5026	864.0016
894.489	908.0369	929.819	1008.7095	1025.2508	1041.8336
1050.9207	1149.544	1193.2542	1240.8722	1252.1471	1271.1128
1310.5477	1355.9063	1390.2383	1414.0686	1453.8702	1455.7505
1474.1843	1702.4503	1727.6967	2964.0945	3027.334	3066.801
3113.3736	3152.6127	3170.7026	3178.9131	3197.064	3219.45

118

Atom	X	Y	Z	(Angstrom)
C	0.02496	0.04283	-0.06169	
C	0.00857	0.08389	1.27762	
C	1.25431	0.01651	2.04165	
C	2.44513	0.15538	1.43815	
C	2.53927	0.46156	-0.05386	
C	1.32351	-0.1241	-0.81019	
C	2.66108	1.95029	-0.17566	
H	3.63293	2.42809	-0.14419	
H	3.44796	0.00048	-0.45311	
H	1.49091	-1.19956	-0.97296	
H	-0.92972	0.15445	1.81789	
H	1.19863	-0.1299	3.1156	
H	3.36682	0.14884	2.01049	
H	1.78478	2.57315	-0.03827	
H	-0.89999	0.07123	-0.6287	

H	1.26215	0.32891	-1.80418

ZPE **0.136783** (Hartree)
CCSD(T)/cc-pVDZ **-271.3772124** (Hartree)

Frequencies cm^{-1}：

146.8319	181.5682	224.0135	330.9715	373.2804	509.5929
551.3466	569.0893	607.299	711.9595	796.5062	802.1667
868.0841	944.461	945.5951	984.8263	1000.7593	1007.958
1033.1887	1097.8365	1120.1731	1173.2326	1202.7424	1245.5705
1304.5096	1343.2173	1355.3584	1394.5845	1440.2822	1456.8616
1471.9629	1665.436	1725.3309	3024.4717	3083.2842	3101.0599
3165.8058	3187.0938	3192.3646	3207.9465	3217.0332	3275.2906

119

Atom	X	Y	Z	(Angstrom)
C	-1.27845	-1.16475	-0.00014	
C	-1.92449	0.03454	-0.00011	
C	-1.20524	1.25491	0.00005	
C	0.21072	1.23644	0.00007	
C	0.92707	0.07249	0.00004	
H	-1.84149	-2.09211	-0.00031	
H	-3.00953	0.05948	-0.00023	
H	-1.73446	2.19964	0.00009	
H	0.74613	2.18183	0.00009	
C	2.42557	0.04124	-0.00002	
H	2.81201	-0.49231	0.87816	
H	2.81195	-0.49167	-0.87862	
H	2.85157	1.04653	0.00033	
C	0.21857	-1.25814	0.0001	
H	0.56056	-1.8557	0.86579	
H	0.56084	-1.85601	-0.86526	

ZPE **0.137194** (Hartree)
CCSD(T)/cc-pVDZ **-271.417837** (Hartree)

Frequencies cm^{-1}：

114.4472	166.4253	261.4187	337.9599	425.1548	495.5457
521.6265	586.7882	667.122	769.6874	771.5177	888.7407
922.4464	941.764	985.5445	987.3617	993.3753	1043.4855
1050.3595	1118.6124	1183.0909	1201.1843	1207.5362	1312.8679
1342.5794	1413.698	1430.2109	1438.0898	1443.9237	1479.8019
1491.7336	1570.5843	1645.5077	2961.636	2962.4282	3036.0201
3083.6609	3142.6318	3186.2864	3193.6329	3211.1129	3233.6113

47-112

Atom	X	Y	Z	(Angstrom)

C	0.24625	1.22083	-0.3724
C	-1.81824	-0.07631	0.09356
C	-1.05421	-1.30819	-0.0573
C	0.29501	-1.28878	-0.10529
C	1.04037	-0.02839	-0.06106
C	2.35521	0.00039	0.20527
H	0.25888	1.36615	-1.47103
H	0.72903	2.10567	0.06376
H	-1.58794	-2.2597	-0.06212
H	-2.88775	-0.13957	0.29812
H	0.86441	-2.22061	-0.12265
H	2.90037	0.9431	0.27597
H	2.91529	-0.92377	0.35971
C	-1.19997	1.12349	0.03848
H	-1.77329	2.04786	0.13317
H	-0.60551	1.22269	2.07745

ZPE **0.129270** (Hartree)

CCSD(T)/cc-pVDZ **-271.3262573** (Hartree)

Frequencies cm^{-1}：

-552.5776	117.799	199.7415	303.8674	374.9903	394.2011
446.7654	486.4621	561.381	604.6384	671.5331	766.6962
783.5921	827.1166	915.4946	938.2056	952.6712	972.5655
993.2993	998.4833	1007.3988	1033.0708	1175.1169	1195.3394
1222.0957	1316.5524	1343.1352	1399.332	1436.8414	1454.9874
1472.2702	1604.6886	1681.3535	1720.3135	3005.2001	3116.4823
3165.0824	3193.8356	3198.8762	3213.5731	3223.8371	3254.0089

47-119

Atom	X	Y	Z	(Angstrom)
C	1.25474	-1.16618	-0.0741	
C	1.8929	0.00231	-0.05806	
C	1.15441	1.2545	0.07836	
C	-0.18527	1.27674	0.06621	
C	-0.9648	0.05602	-0.07679	
H	1.80427	-2.09402	-0.16802	
H	2.96997	0.04227	-0.14803	
H	1.71144	2.17865	0.15552	
H	-0.72415	2.21475	0.11508	
C	-2.28616	0.09378	-0.29424	
H	-2.8573	-0.80882	-0.46674	
H	-2.79956	-0.52218	1.86862	
H	-2.81708	1.03512	-0.34679	
C	-0.23269	-1.25378	0.09754	
H	-0.6545	-2.01432	-0.56133	
H	-0.43188	-1.61172	1.11821	

ZPE	**0.128444**	(Hartree)
CCSD(T)/cc-pVDZ	**-271.3241198**	(Hartree)

Frequencies cm^{-1}：

-294.5162	84.1713	125.1037	186.8805	276.6872	380.7516
438.2523	480.2337	556.2337	593.2975	685.485	761.4295
781.1154	833.4941	908.4682	936.6975	949.4733	968.1566
983.3264	1009.1715	1013.5963	1033.3576	1180.334	1200.8136
1221.2905	1318.0333	1343.9069	1401.5884	1436.4584	1447.0063
1470.5087	1647.575	1671.618	1730.938	2989.9344	3096.2345
3165.3091	3190.9661	3195.395	3210.8717	3221.4079	3254.9396

112-113

Atom	X	Y	Z	(Angstrom)
C	-0.79901	1.03968	0.31364	
C	-2.08237	-0.25315	0.06866	
C	-0.86821	-0.60376	-0.50353	
C	0.13335	-1.4522	-0.07946	
C	1.71462	0.37497	0.07015	
H	-0.74875	0.99494	1.40221	
H	-2.85278	0.24125	-0.5166	
H	-2.43095	-0.67485	1.02191	
H	2.71399	0.75315	0.25217	
H	-1.43362	1.85963	-0.0135	
H	-0.10386	-2.4943	0.12751	
C	1.45486	-0.95798	0.12418	
H	2.24348	-1.65628	0.38435	
C	0.64323	1.37076	-0.24558	
H	0.89838	2.35282	0.18019	
H	0.53526	1.5137	-1.32652	

ZPE	**0.135242**	(Hartree)
CCSD(T)/cc-pVDZ	**-271.2742641**	(Hartree)

Frequencies cm^{-1}：

-547.8907	147.501	243.9748	300.3474	433.0614	465.1594
538.8034	589.2573	629.8979	719.6505	734.7628	782.3027
874.2157	914.2002	960.2407	968.4648	991.6332	997.7738
1078.0566	1078.7686	1146.5202	1183.1303	1196.3852	1216.9249
1296.2518	1335.0371	1347.1875	1432.6979	1441.1899	1471.1247
1490.1537	1541.7559	1629.1997	3029.7545	3032.4956	3078.3398
3090.3309	3170.3536	3173.764	3190.9329	3201.8754	3220.8645

113-114

Atom	X	Y	Z	(Angstrom)
C	0.95017	-0.83103	-0.37458	

C	1.64988	0.10741	0.59965
C	1.02058	1.03512	-0.39569
C	-0.31152	1.52677	-0.0982
C	-1.47817	0.76574	0.07228
C	-1.53609	-0.60698	0.12181
H	1.65564	-1.43069	-0.94858
H	2.73591	0.04183	0.61099
H	1.22167	0.10578	1.60075
H	-2.49649	-1.08746	0.27453
H	0.79696	0.01044	-1.28681
H	-0.38502	2.61008	-0.06828
H	-2.41313	1.30873	0.17791
C	-0.3506	-1.52723	-0.0078
H	-0.56432	-2.27287	-0.78412
H	-0.21679	-2.10463	0.91883

ZPE **0.134250** (Hartree)
CCSD(T)/cc-pVDZ **-271.282367** (Hartree)

Frequencies cm^{-1}：

-834.7994	107.7428	318.1916	365.5988	479.0626	489.4812
534.2839	646.5962	686.3604	749.5259	812.1944	834.1577
883.7134	942.1261	973.3698	976.9286	984.8402	1051.3536
1083.0776	1097.5115	1133.4579	1167.2252	1203.2534	1212.3438
1246.9357	1329.6318	1353.6564	1381.4607	1433.143	1486.1635
1513.3235	1528.9297	1545.73	2247.4289	3032.174	3065.9951
3111.7096	3145.8051	3181.2985	3189.23	3195.0715	3208.9431

114-115

Atom	X	Y	Z	(Angstrom)
C	0.01422	0.01685	0.05587	
C	-0.10146	-0.0039	1.54869	
C	1.68244	-0.24238	2.46193	
C	2.68446	-0.07996	1.52028	
C	2.5289	-0.40892	0.13198	
C	1.34179	-0.4289	-0.51931	
C	0.49027	-1.13202	2.30324	
H	1.33289	-0.6679	-1.5787	
H	3.59611	0.42373	1.82586	
H	0.67349	-2.02853	1.70847	
H	0.00465	-1.37876	3.24631	
H	-0.70617	0.73304	2.0597	
H	-0.77714	-0.61945	-0.38451	
H	-0.20838	1.02714	-0.31794	
H	1.78035	0.26412	3.41736	
H	3.43246	-0.57812	-0.44966	

ZPE **0.136582** (Hartree)

CCSD(T)/cc-pVDZ **-271.361142** (Hartree)

Frequencies cm^{-1}：

-701.2971	139.725	308.4268	348.0966	416.1165	459.8744
532.9563	603.1576	684.1592	769.907	850.4587	860.0838
893.5621	921.3303	944.7152	966.2941	989.6601	1038.7427
1064.7319	1139.7467	1172.8154	1216.2394	1220.091	1231.8962
1239.3827	1350.0606	1363.7961	1403.3393	1449.0804	1460.5405
1484.4651	1526.5375	1664.0931	2950.3573	3035.8199	3096.0702
3164.117	3172.6502	3187.3755	3190.6642	3205.3912	3236.2019

114-118

Atom	X	Y	Z	(Angstrom)
C	-0.00911	0.04423	-0.00144	
C	-0.00316	0.00219	1.35013	
C	1.22376	-0.05982	2.09933	
C	2.44105	0.07574	1.46515	
C	2.51458	0.35381	-0.01169	
C	1.26346	-0.05316	-0.80338	
C	2.65405	1.78029	0.37018	
H	3.62872	2.21088	0.55408	
H	3.41796	-0.0449	-0.47451	
H	1.38217	-1.09062	-1.14958	
H	-0.94263	0.01232	1.89359	
H	1.18589	-0.17064	3.177	
H	3.36936	-0.00862	2.0155	
H	1.775	2.37712	0.5684	
H	-0.94817	0.08015	-0.54386	
H	1.19758	0.55968	-1.70977	

ZPE **0.136494** (Hartree)

CCSD(T)/cc-pVDZ **-271.3666862** (Hartree)

Frequencies cm^{-1}：

-654.6608	175.8334	300.5513	334.3428	479.625	516.671
558.1936	575.9612	658.5726	687.3736	786.5459	819.2885
876.9025	912.5568	936.0031	954.6453	993.7204	1003.7078
1020.4607	1086.9633	1145.0095	1170.8071	1196.5808	1234.8456
1271.6296	1353.255	1366.7	1401.4654	1444.031	1461.7345
1475.0209	1481.5843	1668.3599	3027.5587	3082.8837	3126.5663
3184.8069	3190.3347	3207.2298	3214.9302	3229.5139	3301.3103

115-9

Atom	X	Y	Z	(Angstrom)
C	-0.19222	-0.35492	-0.01766	
C	0.08287	0.45037	1.15362	
C	1.15304	0.33502	1.98158	
C	2.22494	-0.6419	1.8621	

C	2.62357	-1.22072	0.69678
C	2.20937	-0.66646	-0.63839
C	0.73308	-0.92815	-0.81038
H	-1.2417	-0.51073	-0.2546
H	-0.70298	1.13685	1.45781
H	3.70205	0.6626	2.1656
H	1.15698	0.94029	2.88304
H	2.58341	-1.06645	2.79596
H	3.288	-2.07828	0.72629
H	2.78327	-1.12077	-1.44715
H	2.3962	0.41541	-0.65888
H	0.41607	-1.59872	-1.60342

ZPE **0.130546** (Hartree)

CCSD(T)/cc-pVDZ **-271.3272798** (Hartree)

Frequencies cm^{-1}：

-842.4369	210.0964	271.8237	307.2526	358.8986	408.9705
447.4344	465.8005	629.0954	667.2975	747.9417	785.2618
817.484	883.0658	937.9458	945.6776	971.3231	1001.8299
1010.4232	1025.5157	1048.2682	1071.7822	1198.569	1218.7467
1252.3693	1264.7875	1325.8824	1379.783	1418.9732	1472.9114
1480.932	1613.2687	1655.4611	1706.6134	3032.0732	3140.9922
3169.37	3173.932	3181.0936	3194.6772	3202.2792	3206.9759

118-119

Atom	X	Y	Z	(Angstrom)
C	-1.24113	-1.17598	-0.07955	
C	-1.88814	0.00539	-0.08975	
C	-1.17469	1.25291	0.06763	
C	0.19113	1.27446	0.07852	
C	0.95653	0.06218	-0.05597	
H	-1.78469	-2.10766	-0.19546	
H	-2.96376	0.03429	-0.23015	
H	-1.7323	2.17972	0.13193	
H	0.7229	2.22017	0.12943	
C	2.43843	0.03058	-0.02978	
H	2.94962	-0.92035	-0.01308	
H	1.56194	0.07419	-1.13906	
H	3.00424	0.95166	-0.01569	
C	0.23938	-1.25493	0.1899	
H	0.41032	-1.54421	1.24481	
H	0.70269	-2.05544	-0.39877	

ZPE **0.132728** (Hartree)

CCSD(T)/cc-pVDZ **-271.3240302** (Hartree)

Frequencies cm^{-1}：

-1879.0782	123.1292	270.5311	329.5621	425.8827	432.9467
478.2098	553.0213	588.547	619.3908	713.8629	763.1994
785.554	920.8525	937.1185	958.0401	968.8827	996.7112
999.4239	1024.8818	1154.7557	1171.2205	1197.5038	1229.13
1266.4849	1327.2358	1367.1006	1419.265	1442.8454	1463.2332
1486.9456	1581.1489	1698.2028	2228.613	2947.7539	3070.2544
3185.6974	3190.8031	3193.4513	3211.7373	3225.416	3312.3665

119-44

Atom	X	Y	Z	(Angstrom)
C	1.19713	1.18967	−0.0953	
C	1.91317	0.00142	−0.02006	
C	1.23124	−1.21497	0.04733	
C	−0.1664	−1.24074	0.01923	
C	−0.90567	−0.06447	−0.05354	
H	1.71918	2.145	−0.15987	
H	3.0036	0.01807	−0.02625	
H	1.78837	−2.15089	0.10415	
H	−0.69052	−2.19832	0.04824	
C	−2.40711	−0.06415	−0.05359	
H	−2.80605	0.49665	−0.91171	
H	−2.81003	−1.08443	−0.08939	
H	−2.78263	0.42457	0.86069	
C	−0.21005	1.1694	−0.05124	
H	−0.5703	1.60393	1.66939	
H	−0.76539	2.0885	−0.2523	

ZPE	**0.130342**	(Hartree)
CCSD(T)/cc-pVDZ	**-271.3656771**	(Hartree)

Frequencies cm^{-1}：

-879.4332	97.1625	205.0059	287.828	341.9057	406.1268
454.9669	518.2669	528.8662	629.4115	724.1074	754.8363
803.0831	882.4156	956.351	996.0541	1010.488	1017.8941
1039.5122	1058.0531	1069.2824	1106.4697	1177.0042	1197.1869
1238.9522	1318.6948	1346.5358	1413.693	1466.3511	1487.7321
1504.7468	1536.2901	1635.0097	1658.3197	3050.4327	3113.1247
3151.3329	3185.1757	3195.0312	3206.3863	3216.1648	3227.0549

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