

A Combined Crossed Molecular Beam and
Theoretical Investigation of the Elementary
Reaction of Tricarbon ($\text{C}_3(\text{X}^1\Sigma_g^+)$) with
Diacetylene ($\text{C}_4\text{H}_2(\text{X}^1\Sigma_g^+)$): Gas Phase Formation
of the Heptatriynylidyne Radical ($l\text{-C}_7\text{H}(\text{X}^2\Pi)$)

Iakov A. Medvedkov,¹ Anatoliy A. Nikolayev,² Zhenghai Yang,¹ Shane J. Goettl,¹ Alina A. Kuznetsova,² André K. Eckhardt,³ Alexander M. Mebel,^{4*} Ralf I. Kaiser^{1*}

¹ Department of Chemistry, University of Hawai‘i at Manoa, Honolulu, HI 96822, USA

² Samara National Research University, Samara, 443086, Russia

³ Lehrstuhl für Organische Chemie II, Ruhr-Universität Bochum, 44801 Bochum, Germany

⁴ Department of Chemistry and Biochemistry, Florida International University, Miami, Florida, 33199, USA

Corresponding to: ralfk@hawaii.edu; mebel@fiu.edu

Contents

Table S1. Relative energies (E_{rel}) calculated at the different levels of theory, total spin operator expectation values (spin contamination; $\langle S^2_{\text{UHF}} \rangle$), and T1 diagnostic values of intermediates and transition states on the potential energy surface for the bimolecular reaction of the tricarbon $\text{C}_3(\text{X}^1\Sigma_g^+)$ with diacetylene (butadiyne; HCCCCH ; $\text{X}^1\Sigma_g^+$) leading to $\text{C}_7\text{H} + \text{H}$ products.	S3
Figure S1. Potential energy profile for the entrance reaction channel obtained by IRC calculations.	S5
Figure S2. Scanned relaxed potential energy profile from i15 to p1 +H relative to the reactants $\text{C}_3 + \text{C}_4\text{H}_2$ without ZPE energy correction.	S6
Figure S3. Scanned relaxed potential energy profile from i17 to p1 +H relative to the reactants $\text{C}_3 + \text{C}_4\text{H}_2$ without ZPE energy correction.	S7
Figure S4. Scanned relaxed potential energy profile from i19 to p1 +H relative to the reactants $\text{C}_3 + \text{C}_4\text{H}_2$ without ZPE energy correction.	S8
Figure S5. Scanned relaxed potential energy profile from i20 to p1 +H relative to the reactants $\text{C}_3 + \text{C}_4\text{H}_2$ without ZPE energy correction.	S9
Figure S6. (a) Laboratory angular distribution (b) and time-of-flight (TOF) spectra recorded at $m/z = 85$ for the reaction of the tricarbon $\text{C}_3(\text{X}^1\Sigma_g^+)$ with diacetylene $\text{C}_4\text{H}_2(\text{X}^1\Sigma_g^+)$ at a collision energy of $47 \pm 1 \text{ kJ mol}^{-1}$. The best achieved fit for barrierless fit (blue solid lines) mismatch two high-intensity points near the center-of-mass angle on LAD, and also simulated TOF are two fast (37.5°) or two slow (27.75° and 30.25°).	S10
Figure S7. (a) Center-of-mass translational energy $P(E_T)$, (b) angular $T(\theta)$ flux distributions used for barrierless fit for the reaction of the tricarbon $\text{C}_3(\text{X}^1\Sigma_g^+)$ with diacetylene $\text{C}_4\text{H}_2(\text{X}^1\Sigma_g^+)$. Strong forward-scattering feature of $T(\theta)$ function is not aligned with the calculated indirect character of the reactor. The solid blue lines represent the best fit.	S11
Optimized Cartesian coordinates ($\text{\AA}$) and vibrational frequencies (cm^{-1}) for all intermediates, transition states, reactants, and products involved in the $\text{C}_3 + \text{C}_4\text{H}_2$ reactions at the $\omega\text{B97X-D/6-311G(d,p)}$ level.	S12

Table S1. Relative energies (E_{rel}) calculated at the different levels of theory, total spin operator expectation values (spin contamination; $\langle S^2_{\text{UHF}} \rangle$), and T1 diagnostic values of intermediates and transition states on the potential energy surface for the bimolecular reaction of the tricarbon $\text{C}_3(\text{X}^1\Sigma_g^+)$ with diacetylene (butadiyne; HCCCCCH ; $\text{X}^1\Sigma_g^+$) leading to $\text{C}_7\text{H} + \text{H}$ products.

Stationary point	E_{rel} , kJ mol ⁻¹ U ω B97X- D/6- 311G(d,p)	$\langle S^2_{\text{UHF}} \rangle$ U ω B97X- D/6- 311G(d,p)	E_{rel} , kJ mol ⁻¹ CCSD(T)- F12/cc- pVTZ-F12	T1 diagnostic	E_{rel} , kJ mol ⁻¹ CASPT2(12,12)/cc- pVTZ
Intermediates					
<i>i0</i>	-13	0.0	-9	0.018	-
<i>i1</i>	-258	0.0	-225	0.016	-
<i>i2</i>	-52	0.0	-28	0.020	-19 (<i>i1</i>), -32 (<i>i3</i>)
<i>i3</i>	-44	0.0	-21	0.019	-
<i>i4</i>	-56	0.0	-33	0.024	-28 (<i>i1</i>), -40 (<i>i3</i>)
<i>i5</i>	-89	0.0	-70	0.025	-69 (<i>i1</i>)
<i>i6</i>	-84	0.0	-65	0.026	-66 (<i>i1</i>)
<i>i7</i>	-116	0.0	-98	0.018	-
<i>i8</i>	-109	0.0	-100	0.037	-121 (<i>i1</i>), -128 (<i>i7</i>)
<i>i9</i>	-307	0.0	-296	0.026	-335 (<i>i1</i>)
<i>i10</i>	-183	0.0	-170	0.030	-205 (<i>i1</i>), -208 (<i>i14</i>)
<i>i11</i>	-287	0.0	-261	0.025	-280 (<i>i1</i>), -283 (<i>i14</i>)
<i>i12</i>	-316	0.0	-297	0.022	-328 (<i>i1</i>), -331 (<i>i14</i>)
<i>i13</i>	-183	1.0592	-	-	-198 (<i>i1</i>), -201 (<i>i14</i>)
<i>i14</i>	-335	0.0	-309	0.014	-
<i>i15</i>	-350	1.0753	-	-	-283 (<i>i1</i>), -286 (<i>i14</i>)
<i>i16</i>	-214	0.0	-216	0.030	-231 (<i>i1</i>), -234 (<i>i14</i>)
<i>i17</i>	-273	0.0	-252	0.018	-
<i>i18</i>	-113	1.0784	-	-	-74 (<i>i1</i>), -77 (<i>i17</i>), - 73 (<i>i19</i>)
<i>i19</i>	-265	0.0	-242	0.0197	-
<i>i20</i>	-273	0.0	-246	0.022	-258 (<i>i1</i>), -261 (<i>i14</i>), -242 (<i>i17</i>)
Transition states					
<i>i0 – i1 (1)</i>	4	0.0	4	0.019	-
<i>i1 – i2</i>	-23	0.0	2	0.0195	-
<i>i1 – i5</i>	23	0.3908	-	-	34 (<i>i1</i>)
<i>i1 – i6</i>	14	0.5174	-	-	22 (<i>i1</i>)
<i>i1 – i9</i>	-131	0.0	-119	0.018	-
<i>i2 – i3</i>	-16	0.0	0	0.019	-
<i>i2 – i4</i>	-52	0.0	-28	0.021	-20 (<i>i1</i>), -4 (<i>i17</i>)
<i>i3 – i5</i>	-30	0.0	-15	0.019	-
<i>i3 – i17</i>	-43	0.0	-19	0.023	-12 (<i>i1</i>), -24 (<i>i3</i>)
<i>i4 – i17</i>	-56	0.0	-33	0.023	-25 (<i>i1</i>), -9 (<i>i17</i>)
<i>i5 – i7</i>	-70	0.0	-55	0.022	-56 (<i>i1</i>), -63 (<i>i7</i>)

<i>i6 – i7</i>	-65	0.0	-50	0.023	-41 (<i>iI</i>), -48 (<i>i7</i>)
<i>i7 – i8</i>	-98	0.0	-88	0.031	-92 (<i>iI</i>), -100 (<i>i7</i>)
<i>i8 – i15</i>	8	0.0	28	0.035	22 (<i>iI</i>), 15 (<i>i7</i>)
<i>i9 – i10</i>	30	0.0	48	0.027	40 (<i>iI</i>)
<i>i10 – i11</i>	32	0.0	57	0.023	43 (<i>iI</i>), 40 (<i>i14</i>)
<i>i10 – i12</i>	-7	0.0	-2	0.019	-
<i>i11 – i16</i>	33	0.0	23	0.033	-10 (<i>iI</i>)
<i>i12 – i13</i>	-150	0.0	-165	0.019	-
<i>i12 – i14</i>	-183	0.0	-176	0.016	-
<i>i13 – i15</i>	-59	1.0312	-	-	16 (<i>iI</i>), 13 (<i>i14</i>)
<i>i14 – i15</i>	-37	0.0	-13	0.021	27 (<i>iI</i>), 24 (<i>i14</i>)
<i>i15 – i17</i>	6	0.0	28	0.024	48 (<i>iI</i>), 63 (<i>i17</i>)
<i>i15 – i19</i>	34	0.0	42	0.026	45 (<i>iI</i>), 46 (<i>i19</i>)
<i>i15 – i20</i>	5	0.0	30	0.030	37 (<i>iI</i>), 39 (<i>i19</i>)
<i>i16 – i19</i>	-106	0.0	-113	0.022	-113 (<i>iI</i>), -112 (<i>i19</i>)
<i>i17 – i18</i>	-17	0.0	16	0.029	41 (<i>iI</i>), 57 (<i>i17</i>)
<i>i17 – i19</i>	-45	0.0	-41	0.022	-53 (<i>iI</i>), -37 (<i>i17</i>), - 52 (<i>i19</i>)
<i>i17 – i20</i>	48	0.0	52	0.023	43 (<i>iI</i>), 59 (<i>i17</i>)
<i>i18 – i19</i>	24	0.0	56	0.031	82 (<i>iI</i>), 97 (<i>i17</i>), 83 (<i>i19</i>)

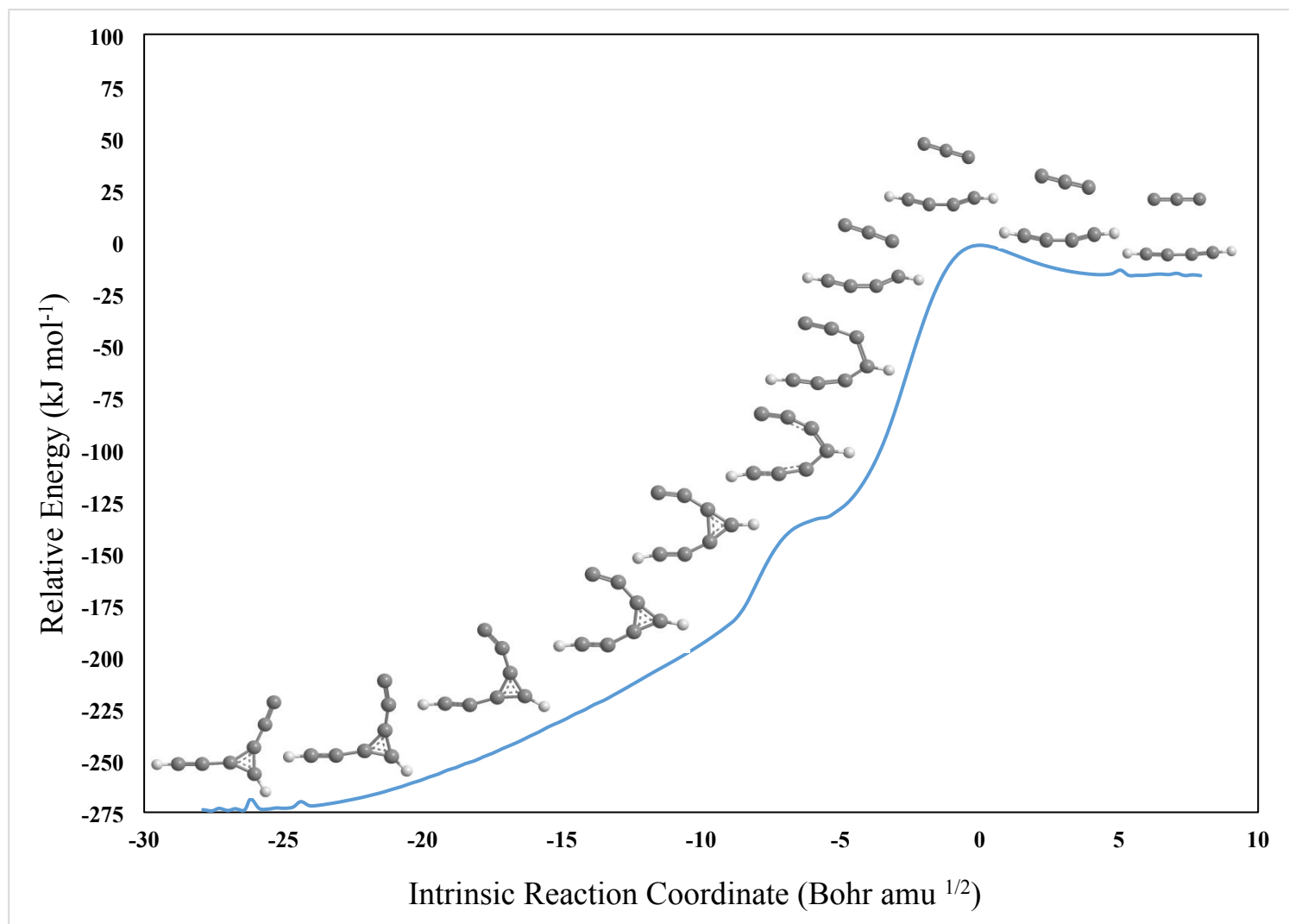


Figure S1. Potential energy profile for the entrance reaction channel obtained by IRC calculations.

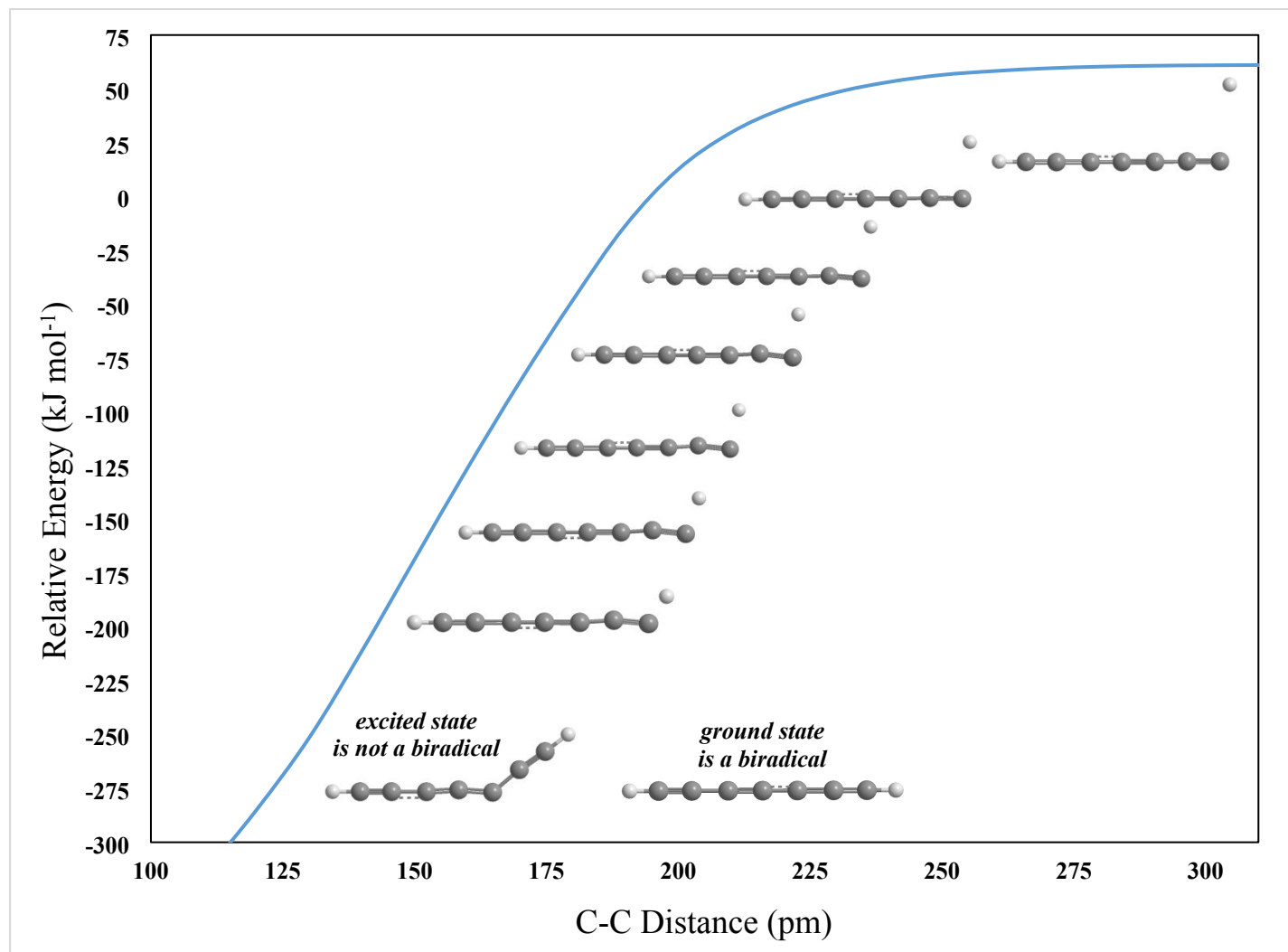


Figure S2. Scanned relaxed potential energy profile from **il5** to **p1**+H relative to the reactants C₃+C₄H₂ without ZPE energy correction.

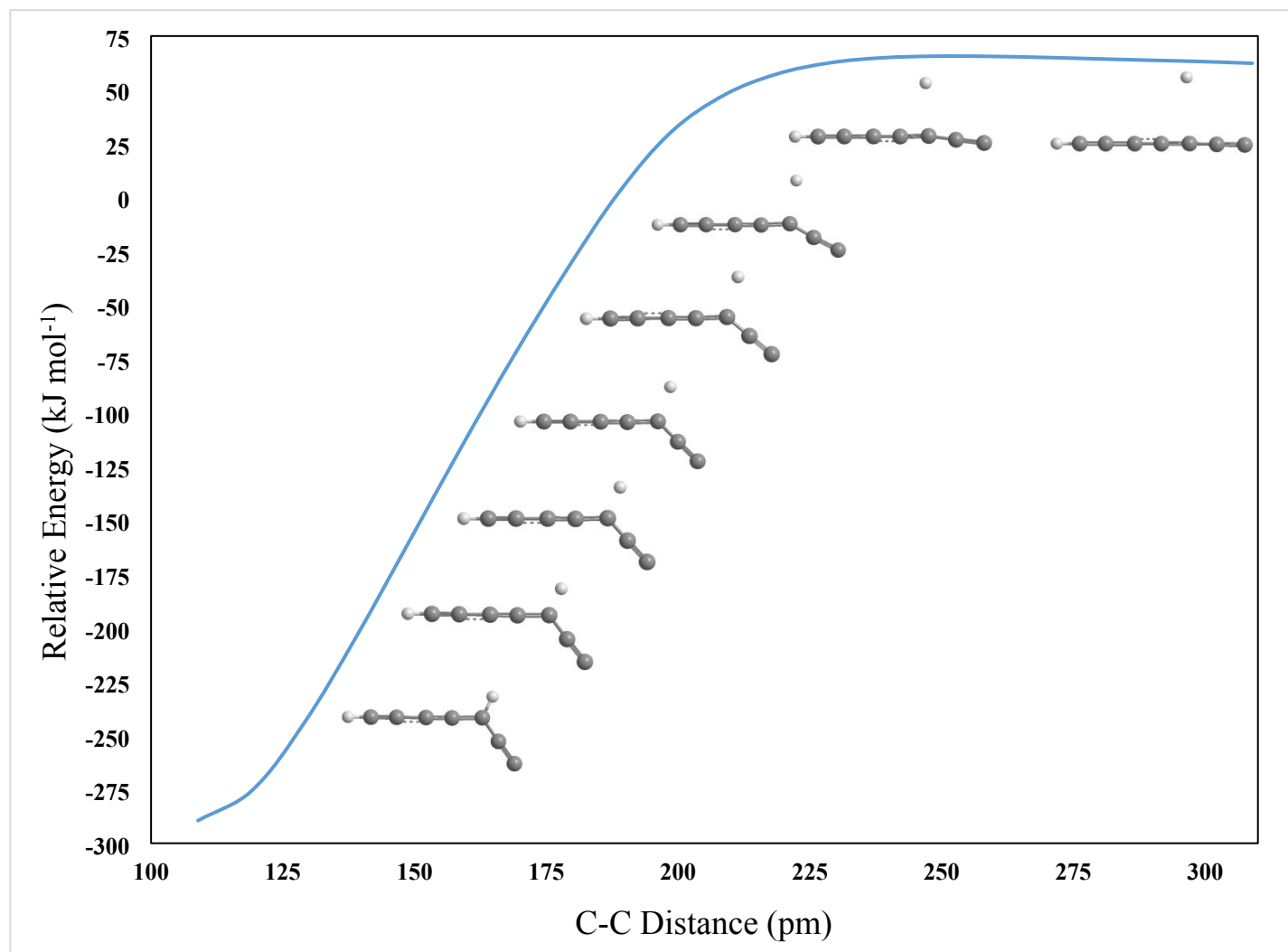


Figure S3. Scanned relaxed potential energy profile from **il7** to **p1**+H relative to the reactants C₃+C₄H₂ without ZPE energy correction.

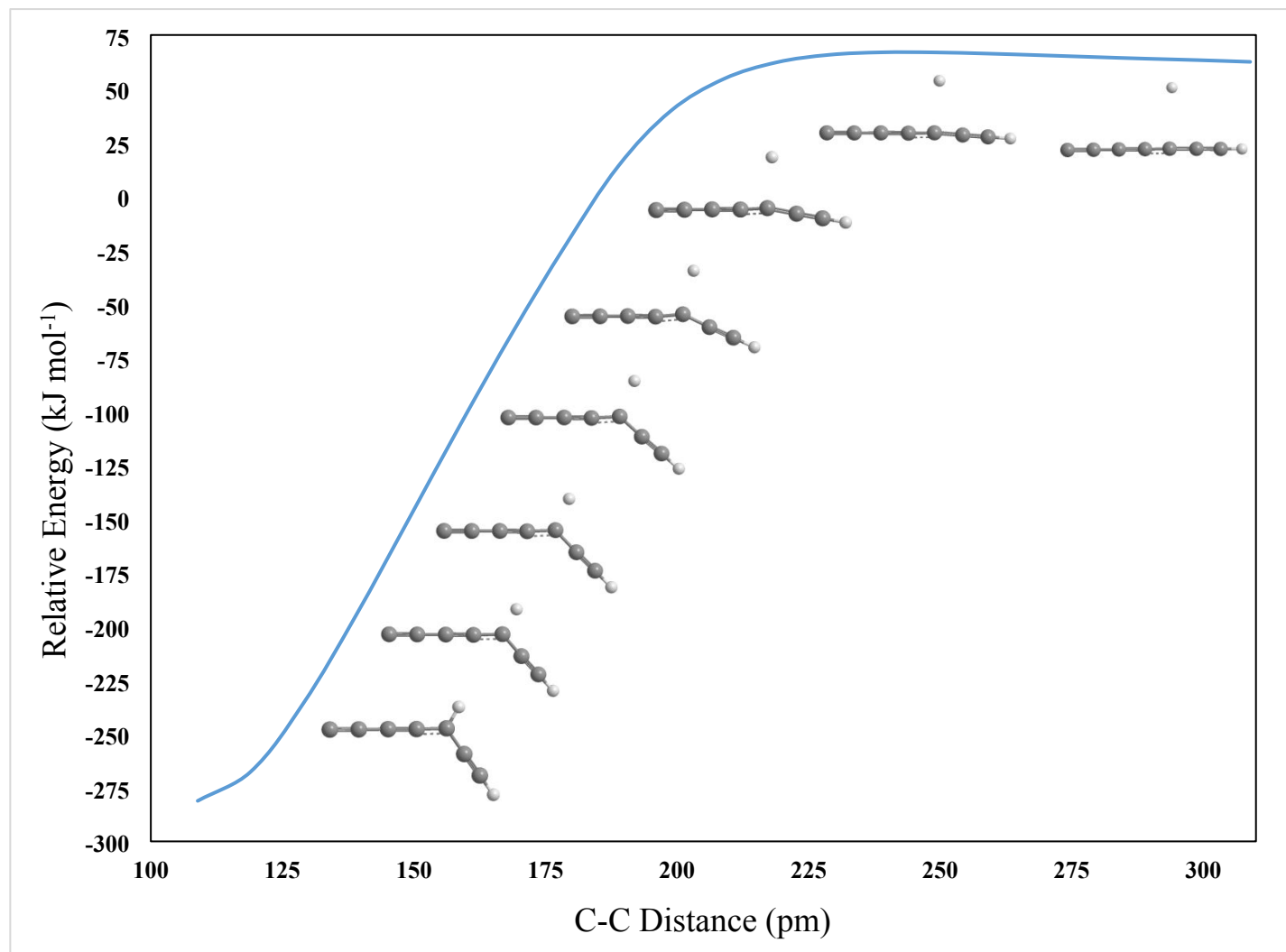


Figure S4. Scanned relaxed potential energy profile from **i19** to **p1**+H relative to the reactants C₃+C₄H₂ without ZPE energy correction.

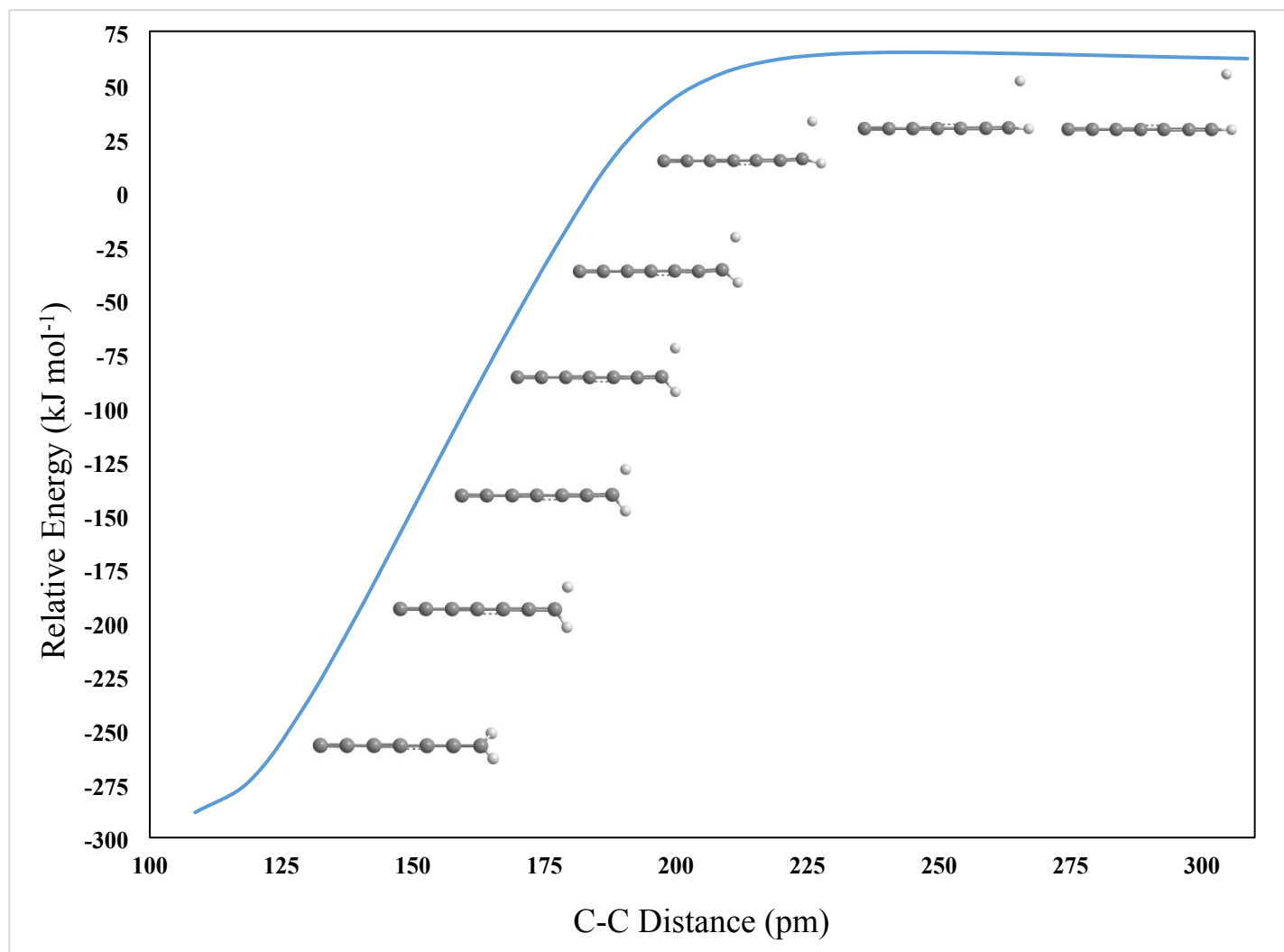


Figure S5. Scanned relaxed potential energy profile from **i20** to **p1**+H relative to the reactants C₃+C₄H₂ without ZPE energy correction.

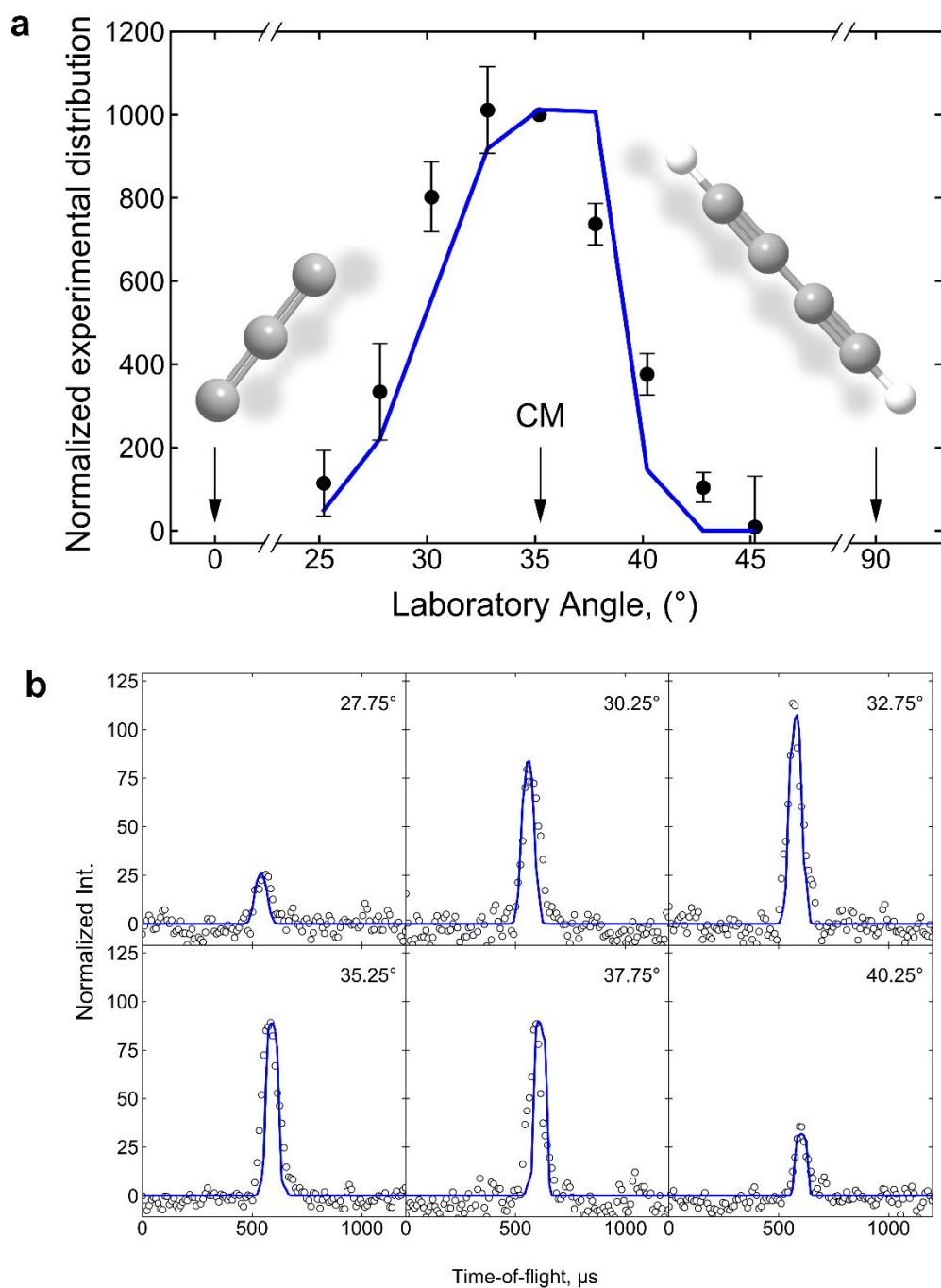


Figure S6. (a) Laboratory angular distribution (b) and time-of-flight (TOF) spectra recorded at $m/z = 85$ for the reaction of the tricarbon $C_3(X^1\Sigma_g^+)$ with diacetylene $C_4H_2(X^1\Sigma_g^+)$ at a collision energy of 47 ± 1 kJ mol $^{-1}$. The best achieved fit for barrierless fit (blue solid lines) mismatch two high-intensity points near the center-of-mass angle on LAD, and also simulated TOF are two fast (37.5°) or two slow (27.75° and 30.25°). The circles represent the experimental data.

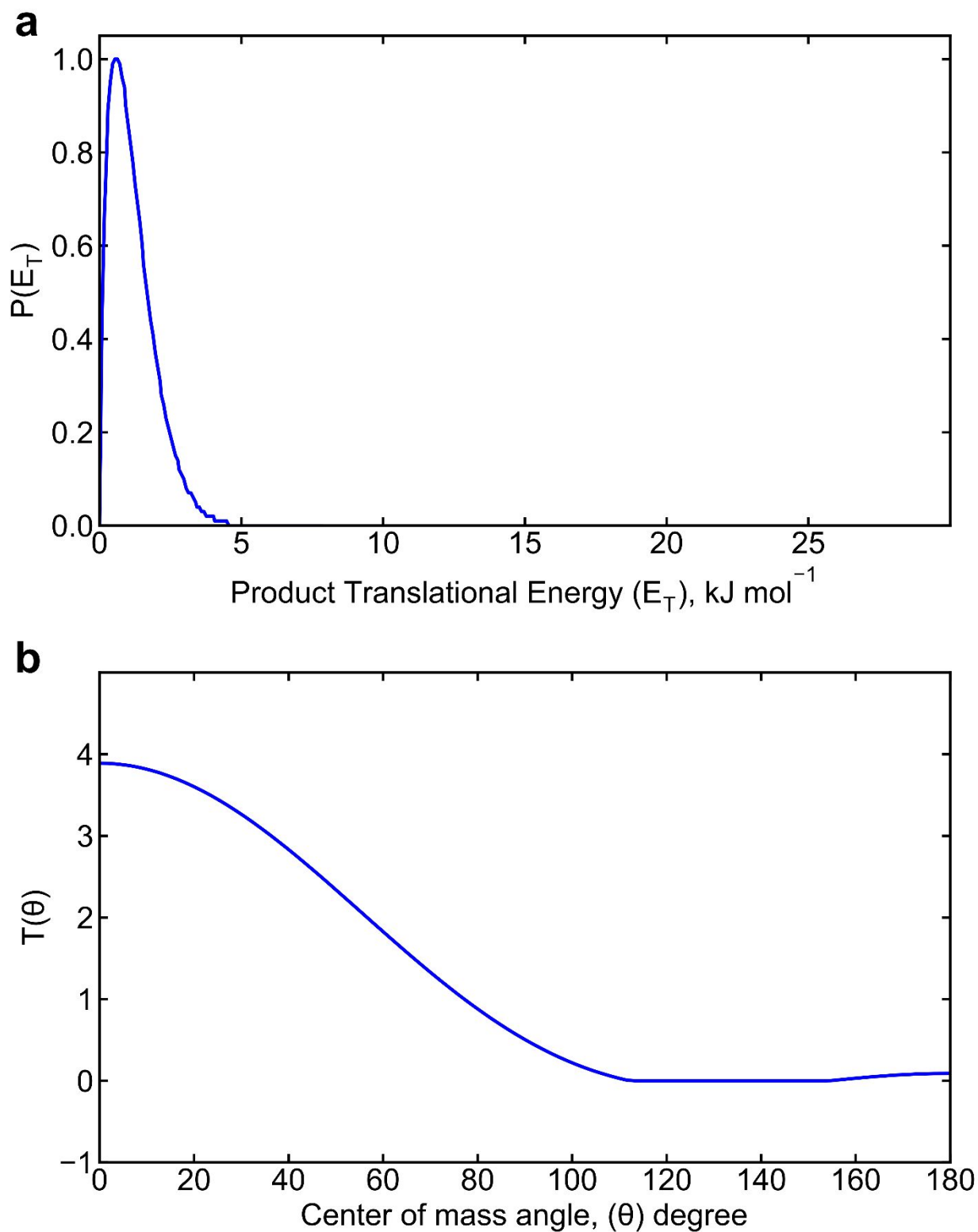


Figure S7. (a) Center-of-mass translational energy $P(E_T)$, (b) angular $T(\theta)$ flux distributions used for barrierless fit for the reaction of the tricarbon $\text{C}_3(\text{X}^1\Sigma_g^+)$ with diacetylene $\text{C}_4\text{H}_2(\text{X}^1\Sigma_g^+)$. Strong forward-scattering feature of $T(\theta)$ function is not aligned with the calculated indirect character of the reactor. The solid blue lines represent the best fit. For $T(\theta)$, the direction of the tricarbon beam is defined as 0° and of the diacetylene as 180° .

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) for all intermediates, transition states, reactants, and products involved in the C₃ + C₄H₂ reactions at the ωB97X-D/6-311G(d,p) level.

Reactants

C₃

Cartesian coordinates

C	-0.486711	0.188336	0.000000
C	-1.774828	0.188336	-0.000000
C	0.801406	0.188336	0.000000

Vibrational frequencies

91.8051	91.8051	1258.7608
2174.2960		

C₄H₂

Cartesian coordinates

C	-1.283592	0.171431	-0.000000
C	0.089865	0.171431	0.000000
C	1.291675	0.171431	0.000000
C	-2.485402	0.171431	-0.000000
H	-3.548993	0.171431	-0.000000
H	2.355266	0.171431	0.000000

Vibrational frequencies

228.6419	228.6419	533.6499
533.6499	691.5827	691.5827
692.5100	692.5100	911.9949
2143.9236	2336.7416	3482.5932
3482.9776		

Intermediates

i0

Cartesian coordinates

C	-1.210335	-0.888431	0.263662
C	-1.371595	0.450645	0.498060
C	-1.435516	1.638231	0.680773
C	-0.991432	-2.049359	0.035281
H	-0.812850	-3.079347	-0.162368
H	-1.507223	2.686603	0.846929
C	1.579893	1.561217	-0.289212
C	1.728523	0.300477	-0.508880
C	1.883416	-0.959186	-0.730394

Vibrational frequencies

65.3463	85.4530	98.0665
112.3578	134.4981	220.5371
233.0438	241.4187	535.8692
537.7390	714.6434	715.3818
717.5284	718.8429	919.3057
1261.2689	2133.1294	2163.4991
2326.1311	3483.3764	3483.5675

i1

Cartesian coordinates

C	-0.124879	0.445902	0.649071
C	-0.024518	0.088642	-0.692818
C	0.052549	-0.185753	-1.858649

C	-0.034141	0.123876	1.944188
H	0.178283	-0.630901	2.684327
H	0.121052	-0.429656	-2.892990
C	-0.404248	1.439281	1.630847
C	-0.754127	2.683031	1.957009
C	-1.085979	3.862728	2.256817

Vibrational frequencies

95.8844	145.1951	200.5968
207.6268	401.7239	410.2847
585.7503	603.5368	690.5339
709.8532	766.6902	822.4107
857.9586	1013.1863	1153.5564
1486.7955	1777.7458	2113.1784
2256.5200	3291.5194	3473.9579

i2

Cartesian coordinates

C	-0.216421	0.309354	-0.846030
C	-1.349740	0.077305	0.032017
C	-2.185711	-0.161463	0.873759
C	1.187461	0.134212	-0.605572
H	1.834203	0.384199	-1.444184
H	-2.927697	-0.369269	1.609047
C	1.690213	-0.299934	0.546944
C	2.155004	-0.718159	1.660939
C	-1.176499	0.657931	-1.667373

Vibrational frequencies

56.6752	112.0140	150.6059
244.1925	256.2176	276.0749
349.6522	481.8632	556.0643
594.9485	773.7477	852.7810
897.7281	1073.5230	1179.5800
1388.8365	1763.0727	2063.2575
2123.1771	3168.1731	3470.6746

i3

Cartesian coordinates

C	0.340608	0.209536	-0.070590
C	1.774974	0.035129	-0.059945
C	2.977785	-0.070021	-0.062791
C	-0.688522	-0.754280	0.233469
H	-0.341441	-1.748568	0.508688
H	4.038169	-0.167242	-0.064012
C	-1.990530	-0.482915	0.191300
C	-3.247581	-0.255333	0.160337
C	0.548660	1.458844	-0.433872

Vibrational frequencies

40.2207	102.0116	138.9990
191.3984	229.4075	262.4426
376.3937	469.3887	494.7250
573.5583	822.8415	897.8450
901.7537	1055.4294	1176.7031
1428.0588	1724.7383	2063.8045
2156.7695	3161.7092	3470.9950

i4

Cartesian coordinates

C	0.458314	-0.947194	-0.004950
C	1.472829	0.275910	-0.005543

C	1.435880	1.491943	-0.001587
C	-0.951720	-0.967381	0.001117
H	-1.386342	-1.966775	-0.000112
H	1.381200	2.555595	0.001970
C	-1.712448	0.128109	0.007843
C	-2.403001	1.201553	0.014196
C	1.719420	-1.231405	-0.011319

Vibrational frequencies

88.2928	122.8640	204.6913
257.2656	263.9748	310.7154
377.8211	445.6023	581.0949
609.4981	760.1887	791.2900
880.6308	940.5227	1145.0909
1384.4086	1809.5671	2054.4804
2066.9890	3146.0094	3465.8597

i5

Cartesian coordinates

C	-0.079900	0.832735	0.411767
C	0.011132	0.249873	-0.860846
C	0.135241	-0.235514	-1.951337
C	0.046314	0.425842	1.732932
H	-0.215856	-0.514226	2.210636
H	0.238771	-0.664729	-2.919723
C	-0.077038	1.746532	2.340100
C	0.435645	2.348543	3.367198
C	-0.833830	1.864882	1.016154

Vibrational frequencies

120.2850	141.3315	213.1306
273.3547	479.8102	515.1181
530.1091	622.1038	704.0375
718.0480	746.6391	817.2200
923.9160	1005.5660	1205.7283
1227.4007	1590.4086	1818.3433
2256.6660	3180.1272	3478.9071

i6

Cartesian coordinates

C	0.255123	-0.255245	0.133442
C	0.036070	-1.115500	-0.966866
C	-0.086671	-1.848799	-1.908994
C	0.257287	-0.479882	1.505267
H	0.457834	-1.318756	2.151953
H	-0.207130	-2.496126	-2.745481
C	-0.641583	0.595671	1.522502
C	-0.076590	1.175247	0.215220
C	0.248421	2.241816	-0.445888

Vibrational frequencies

130.0769	182.1241	221.7209
261.5002	395.4653	545.1516
603.3397	656.1483	734.0115
759.5020	765.9521	796.1869
863.7897	1045.3509	1134.8088
1319.7108	1486.1769	1811.7412
2242.9768	3282.1394	3476.3975

i7

Cartesian coordinates

C	-0.169051	0.485769	0.446241
---	-----------	----------	----------

C	-0.014968	-0.012729	-0.858852
C	0.113670	-0.424531	-1.979580
C	-0.031241	0.060900	1.700834
H	0.166971	-0.870693	2.211768
H	0.228856	-0.792164	-2.971805
C	-0.287439	1.445734	2.259380
C	-0.691619	2.772372	2.012702
C	-0.586502	1.896032	0.907773

Vibrational frequencies

61.4965	156.6818	234.0819
332.7138	376.4021	494.2058
579.5334	626.4847	712.8493
739.2766	792.3196	845.1083
949.2851	1060.1748	1129.2405
1200.6008	1576.3489	1707.8948
2246.8279	3246.9467	3477.7087

i8

Cartesian coordinates

C	-0.062387	0.800612	0.402119
C	-0.009219	0.150055	-0.850086
C	0.084875	-0.411398	-1.907959
C	-0.102627	0.206325	1.707011
H	-0.144548	-0.848615	1.944277
H	0.160476	-0.903921	-2.848024
C	-0.595662	1.302749	2.444098
C	-0.140970	2.487835	1.963321
C	-0.551110	2.099367	0.737554

Vibrational frequencies

139.6189	169.3196	307.3518
357.2186	520.6050	579.2240
631.1380	675.9432	685.6882
732.4270	843.7025	901.7768
996.1381	1117.4629	1237.3954
1284.1104	1326.5995	1441.3222
2239.9654	3244.2940	3480.2378

i9

Cartesian coordinates

C	0.082263	-0.485928	0.992955
C	0.075880	-0.289678	-0.248389
C	-0.071171	0.726551	-1.167569
C	-0.053984	0.197021	2.182185
H	-0.000221	-0.256174	3.164863
H	-0.027970	0.598635	-2.242605
C	-0.276811	1.586671	1.975875
C	-0.316728	1.985760	0.749519
C	-0.289780	1.984438	-0.540475

Vibrational frequencies

259.6486	354.9597	376.6233
503.0852	567.0884	568.4078
584.3081	682.4637	905.1230
911.9088	943.8764	994.9258
1165.1063	1299.8160	1311.2717
1376.5563	1437.3897	1813.3777
2000.9764	3206.5283	3207.5144

i10

Cartesian coordinates

C	-1.479691	-0.897880	-0.000001
C	-0.168473	-1.364486	-0.000002
C	0.937547	-0.520182	-0.000001
C	-1.604523	0.562190	0.000000
C	-0.414798	1.171988	0.000000
C	0.854538	0.951238	0.000000
C	2.088346	0.219531	0.000000
H	0.026647	-2.433396	-0.000002
H	-2.569986	1.052442	0.000000

Vibrational frequencies

219.0585	267.3005	359.9976
499.7842	542.0990	569.0460
639.8913	806.7017	855.3358
865.5694	887.2294	955.4099
987.6275	1212.2477	1230.3801
1347.1073	1408.5045	1596.9128
1870.8741	3186.8468	3218.1784

ii1

Cartesian coordinates

C	1.600712	0.429253	-0.000041
C	0.498328	1.279108	0.000054
C	-0.777169	0.700374	0.000067
C	1.403101	-1.001115	-0.000129
C	0.157985	-1.245663	-0.000084
C	-1.043621	-0.702724	-0.000004
C	-2.106448	0.276088	0.000073
H	2.595579	0.865015	-0.000053
H	0.631644	2.352812	0.000118

Vibrational frequencies

208.9303	408.2504	432.8125
492.9839	524.0063	621.2152
656.4579	785.3250	827.9014
953.0158	997.7721	1027.2952
1099.2788	1178.5349	1364.5402
1425.4609	1450.7546	1658.4631
1845.8618	3194.3387	3240.2372

ii2

Cartesian coordinates

C	0.873122	0.900976	-0.000019
C	1.421382	-0.248904	0.000005
C	0.713246	-1.437327	0.000031
C	0.002213	1.956264	-0.000041
H	-1.211021	-2.403214	0.000052
H	1.205595	-2.405944	0.000052
C	-0.871078	0.902946	-0.000019
C	-1.421934	-0.245692	0.000005
C	-0.716484	-1.435712	0.000031

Vibrational frequencies

290.0967	395.6668	440.4073
504.3594	510.8876	548.4136
608.5483	733.9013	875.5239
943.8659	992.6297	1011.8335
1111.9813	1288.3807	1340.4129
1377.9458	1470.0255	1817.4400
1870.5356	3181.1359	3197.9477

ii3

Cartesian coordinates

C	1.289155	-1.120521	0.064955
C	1.525338	0.230054	0.076341
C	0.703270	1.344341	0.035267
C	0.001480	-1.288708	0.000241
C	-1.286771	-1.124410	-0.064642
C	-1.525653	0.225738	-0.075838
C	-0.706843	1.342212	-0.034589
H	1.179044	2.321724	0.058776
H	-1.184514	2.318669	-0.057688

Vibrational frequencies

150.0024	239.7338	297.3835
482.2151	509.6198	595.2982
647.6123	807.7083	809.1937
955.5770	1009.3368	1088.9700
1135.4982	1258.6767	1397.6355
1421.4321	1520.2505	1606.3034
1773.6224	3167.8398	3183.7883

ii4**Cartesian coordinates**

C	-0.689810	0.412860	0.011466
C	-1.843830	-0.369224	-0.005069
C	-2.841798	-1.037396	-0.019159
C	-0.084019	1.700659	0.041617
H	3.868616	-1.253216	-0.039409
H	-3.727341	-1.627442	-0.031592
C	0.645339	0.478630	0.010092
C	1.870601	-0.186255	-0.008890
C	2.929384	-0.753087	-0.025096

Vibrational frequencies

97.3652	178.0965	232.7766
238.8551	451.8507	469.6390
576.7681	616.0925	668.3748
669.3250	696.7616	770.7445
772.5133	798.1185	1249.3822
1263.1641	1815.4065	2239.5596
2246.1371	3477.6329	3478.0005

ii5**Cartesian coordinates**

C	1.378643	0.079054	-0.000056
C	2.679340	-0.194287	-0.000126
C	3.872192	-0.444593	-0.000107
C	-3.594340	1.125888	0.000033
C	-2.401759	0.874092	0.000014
C	-1.101190	0.600200	0.000093
C	0.138639	0.339277	-0.000016
H	4.913037	-0.662963	-0.000039
H	-4.634927	1.345590	0.000117

Vibrational frequencies

77.4082	187.2976	192.4553
402.1409	403.2331	497.6654
497.7277	563.4815	603.2534
604.0742	608.0148	608.0181
665.5287	674.9703	1077.3235
1559.5699	1709.0102	2078.1061
2114.7038	3471.7380	3474.3510

i16**Cartesian coordinates**

C	-1.603481	0.220866	-0.244966
C	-0.653984	1.159216	-0.058866
C	0.644918	1.427819	0.143164
C	-0.979394	-0.968871	0.148727
C	0.120382	-1.575237	0.274381
C	1.149242	-0.821373	-0.157813
C	1.563121	0.357408	-0.200339
H	-2.482406	0.294552	-0.873746
H	0.987633	2.320629	0.654859

Vibrational frequencies

272.7247	331.0687	369.4963
407.4011	433.3673	471.2510
488.5036	601.2311	824.8850
845.7993	1017.8298	1039.4466
1095.1954	1292.7118	1328.4020
1343.3422	1735.0480	1811.8853
1937.7556	3192.8327	3198.6983

i17**Cartesian coordinates**

C	1.151787	0.214036	0.013855
C	2.476986	-0.113300	0.001918
C	3.644573	-0.401972	-0.008610
C	-3.366769	-0.847479	-0.030018
H	4.677607	-0.658050	-0.017951
C	-2.386455	-0.028277	0.002358
C	-1.384179	0.852378	0.037160
C	-0.024969	0.493783	0.024030
H	-1.600610	1.920630	0.078528

Vibrational frequencies

76.6355	132.9200	185.4776
231.5928	313.2199	317.6963
499.6295	554.6495	569.5939
704.6941	734.4634	777.6881
892.3548	1109.5285	1234.1811
1434.2839	2054.1103	2198.5661
2359.2934	3131.4800	3478.3544

i18**Cartesian coordinates**

C	-1.224184	0.310884	0.731074
C	-2.309609	-0.068777	0.101103
C	-3.366869	-0.394960	-0.437127
C	0.040798	0.543200	1.101112
C	1.127022	0.133652	0.365046
C	2.125307	-0.239783	-0.306299
C	3.156794	-0.631147	-1.009512
H	0.260578	1.080494	2.025249
H	-4.271662	-0.684450	-0.915615

Vibrational frequencies

33.5818	133.3194	135.0148
220.3679	270.3775	351.1999
394.5183	463.6174	469.1813
570.6884	631.5788	731.7187
827.0524	917.3289	1287.5626
1513.3856	1576.5416	1867.9621
2015.1129	3109.2842	3468.9672

i19**Cartesian coordinates**

C	1.207211	-0.851147	-0.000472
C	2.287212	0.061801	-0.000305
C	3.225131	0.812988	-0.000210
C	-0.065621	-0.482973	-0.000230
C	-1.280774	-0.158841	-0.000037
C	-2.535002	0.180797	0.000131
C	-3.768888	0.512434	0.000111
H	4.048049	1.488236	-0.000122
H	1.457164	-1.911312	-0.000826

Vibrational frequencies

69.6953	125.1948	183.2462
262.7571	298.7030	330.3860
479.5337	537.5873	590.2790
716.3181	746.3431	812.5944
863.3261	1029.4497	1282.5486
1516.0474	2013.7756	2215.0242
2263.6845	3143.2157	3478.3722

i20**Cartesian coordinates**

C	0.909635	0.098792	-0.006818
C	2.160331	-0.091970	-0.036124
C	3.455328	-0.289462	-0.066426
C	-4.152232	0.871886	0.111873
C	-2.889590	0.678811	0.082245
C	-1.608494	0.483156	0.052208
C	-0.361006	0.292640	0.022978
H	3.892429	-1.200916	0.331013
H	4.125483	0.453128	-0.489763

Vibrational frequencies

66.4835	75.9801	168.4484
192.8018	289.3712	293.3819
457.5485	547.4523	559.9617
576.3374	687.4564	960.1160
1025.2026	1090.3730	1429.3498
1597.0956	1980.5652	2206.4982
2237.1364	3140.0928	3229.7486

Transition states***i14 – i15*****Cartesian coordinates**

C	-0.577837	1.244583	0.018481
C	-1.441656	0.078415	-0.000955
C	-2.168141	-0.880195	-0.016913
C	-1.496480	2.197250	0.036163
C	0.855438	1.375343	0.019177
C	1.562422	0.205052	-0.002074
C	2.292451	-0.771085	-0.019955
H	-2.798217	-1.737677	-0.031210
H	2.937141	-1.617633	-0.035475

Vibrational frequencies

-285.4615	84.1966	87.7111
209.4852	241.4848	326.8963
419.1020	444.4814	558.0492
610.9633	641.6680	767.3942
782.2553	855.7318	1004.8441

1262.8568	1671.6173	2062.6865
2197.9208	3472.3535	3479.7632

i18 – i19

Cartesian coordinates

C	1.001941	0.391794	0.499993
C	2.143182	-0.303546	0.156703
C	3.207259	-0.838595	-0.053686
C	-0.259912	0.134321	0.123738
C	-1.536293	-0.044631	0.075993
C	-2.808127	-0.227455	-0.005662
C	-4.080858	-0.413027	-0.078504
H	0.254775	1.073719	-0.492103
H	4.132295	-1.327021	-0.250028

Vibrational frequencies

-1278.0210	80.4049	108.5294
171.6550	244.9603	298.1986
371.2539	416.6159	483.0237
557.4418	560.9456	705.1980
798.2978	826.8113	1045.8843
1456.0584	1893.5887	2132.4277
2186.7235	2297.4419	3473.9744

i1 – i6

Cartesian coordinates

C	0.190522	-0.114090	0.442859
C	-0.009727	-0.687154	-0.792573
C	-0.131650	-1.161609	-1.891614
C	0.239153	-0.150098	1.754757
C	-0.536856	1.015919	1.545963
C	-0.338627	1.794323	0.436113
C	-0.050660	2.645402	-0.483813
H	-0.250345	-1.579713	-2.863324
H	0.463670	-0.782170	2.595363

Vibrational frequencies

-575.6489	117.9568	171.5053
214.6242	278.0449	400.5121
448.2824	492.2731	536.7364
707.4048	739.9996	760.3083
812.6809	951.4699	1112.2758
1190.5844	1726.9825	1841.0997
2214.5984	3308.8589	3474.6580

i16 – i19

Cartesian coordinates

C	0.942457	0.780437	0.007221
C	1.763382	-0.347434	0.018881
C	1.912248	-1.595512	0.008243
C	-0.387110	0.464318	0.185791
C	-0.876380	-0.705192	0.134278
C	-0.744931	-1.964228	-0.127023
C	0.275890	-2.765854	-0.130071
H	1.311236	1.775998	-0.215329
H	2.622862	-2.388264	0.117847

Vibrational frequencies

-467.0382	160.9088	261.4282
286.3001	399.5601	433.4732
484.0812	537.9629	607.9866
720.7553	882.2727	903.3820

1053.9109	1064.4327	1342.4342
1397.7764	1752.5830	1870.7670
1956.9948	3193.0629	3387.9022

i17 – i20

Cartesian coordinates

C	1.158325	-1.750780	0.129687
C	2.270161	-1.031023	0.063732
C	2.540603	0.194813	-0.039548
C	-2.131817	1.948176	-0.159064
C	-1.267391	1.009736	-0.085972
C	-0.308415	0.116761	-0.017182
C	0.032932	-1.186226	0.089092
H	3.301138	0.949122	-0.106413
H	1.130177	0.546387	-0.060872

Vibrational frequencies

-1571.3111	121.0723	134.3517
261.7966	328.3764	441.7735
459.1278	524.6154	540.2296
555.4632	723.9900	878.1650
902.5008	1041.8199	1290.4979
1477.6431	1522.2569	1897.6434
1931.4687	2089.2959	3355.8990

i15 – i19

Cartesian coordinates

C	0.582050	-0.536872	0.058063
C	1.946959	-0.717871	0.174255
C	3.123630	-0.955241	0.266715
C	-1.836010	-2.209430	-0.335667
C	-2.131597	-0.951570	-0.245812
C	-1.647006	0.244805	-0.085102
C	-0.354032	0.352088	0.050940
H	4.166521	-1.151770	0.349975
H	-0.393251	-1.664242	-0.143829

Vibrational frequencies

-1622.1768	110.9260	139.6498
200.7662	333.5837	357.2122
473.4084	500.8675	552.9424
589.0825	685.5038	765.8936
900.2106	1029.1866	1236.2197
1384.9449	1544.5220	1730.7085
1876.2923	2227.6838	3477.1325

i11 – i16

Cartesian coordinates

C	-1.374781	-0.731090	0.155618
C	-0.051050	-1.221460	0.025461
C	1.151900	-0.714725	-0.094472
C	-1.351011	0.653918	0.151747
C	-0.222332	1.309843	0.039645
C	1.027951	1.209461	-0.083844
C	2.135869	0.358780	-0.193916
H	-2.243636	-1.368170	0.242361
H	1.109170	-2.006688	-0.090033

Vibrational frequencies

-1585.1656	34.0954	289.0546
366.4425	470.7303	503.8121
557.9528	568.1480	645.7837

657.9558	690.7070	863.3282
977.3322	1033.5545	1210.5686
1273.8455	1481.3115	1759.2523
1940.9297	2179.9002	3251.4286

i17 – i19

Cartesian coordinates

C	-1.274309	-0.767430	0.169279
C	-0.039320	-1.350651	-0.022430
C	1.200664	-1.413289	-0.202664
C	-1.187483	0.623431	0.186793
C	-0.213743	1.387064	0.062932
C	1.083411	1.596106	-0.119645
C	2.110962	0.906018	-0.283076
H	-2.197625	-1.324703	0.291477
H	2.199603	-0.359526	-0.323776

Vibrational frequencies

-1316.4849	129.6460	285.5978
288.6912	338.4004	400.1327
415.0073	473.2837	496.7282
599.9384	915.1125	997.3914
1003.9956	1085.5235	1317.2808
1389.8817	1626.3162	1980.6050
2046.4583	2081.3785	3196.3372

i9 – i10

Cartesian coordinates

C	0.280705	-1.564434	0.513096
C	0.219376	-0.919244	-0.647835
C	0.051794	0.167349	-1.293956
C	0.045483	-0.555867	1.535026
C	-0.178862	0.765096	1.169147
C	-0.235924	1.373194	0.060102
C	-0.202449	1.557998	-1.311034
H	0.301203	-0.995222	-2.029193
H	0.051754	-0.868313	2.574118

Vibrational frequencies

-1539.1311	195.6427	363.4499
476.8747	487.8741	533.2370
568.7468	617.2606	645.0221
758.1745	827.7321	914.9421
963.0612	1060.6683	1294.0683
1298.5654	1348.5984	1845.0186
1905.7818	2018.6823	3198.9392

i5 – i7

Cartesian coordinates

C	0.018129	0.204065	-0.233500
C	0.058956	-0.432340	-1.483465
C	0.138178	-0.967049	-2.555132
C	0.144164	-0.190210	1.109512
C	0.106378	1.080787	1.728606
C	0.004713	2.319541	2.055583
C	-0.701723	1.268026	0.329429
H	0.202588	-1.435630	-3.508425
H	-0.199699	-1.109163	1.577089

Vibrational frequencies

-230.1414	128.5634	170.6041
258.9741	428.5483	505.4583

522.1462	627.4452	634.5837
701.6035	740.7600	811.2707
923.1331	1041.0460	1211.0202
1240.7887	1563.4941	1915.8282
2254.3706	3179.3907	3480.9409

i15 – i20

Cartesian coordinates

C	0.817878	0.641121	0.000477
C	1.486200	-0.470545	-0.220984
C	1.713528	-1.704325	-0.443017
C	-1.059312	-2.232299	-0.405421
C	-1.539039	-1.078695	-0.185501
C	-1.746292	0.263181	0.054111
C	-0.451560	0.602368	0.052498
H	2.592891	-2.310228	-0.587580
H	0.550040	-2.172216	-0.469439

Vibrational frequencies

-997.8765	181.9423	190.7012
330.5258	350.8609	391.9667
433.4677	503.7425	600.3517
684.1294	684.3533	878.8813
1012.2181	1052.3272	1094.7702
1277.0801	1430.5138	1803.4338
1889.3825	1945.2251	3301.7965

i13 – i15

Cartesian coordinates

C	1.214754	1.584615	-0.422549
C	1.479154	0.265783	-0.213795
C	1.093253	-0.913026	-0.008107
C	0.011520	1.823833	0.001177
C	-1.188882	1.570791	0.424907
C	-1.438467	0.249237	0.215224
C	-1.039388	-0.925031	0.008724
H	1.384486	-1.917144	0.225116
H	-1.319408	-1.932181	-0.225165

Vibrational frequencies

-604.7937	153.4396	223.5328
374.8175	447.5321	459.6283
493.9955	503.9319	584.8692
638.5364	652.5844	763.6930
847.5083	1044.2889	1105.3872
1336.6965	1598.9554	1785.5235
1913.1571	3373.0865	3373.9715

i3 – i17

Cartesian coordinates

C	-0.256559	0.316183	-0.114469
C	-1.767484	0.167447	-0.107841
C	-2.821194	-0.428953	-0.002257
C	0.763520	-0.659957	0.101817
H	0.428975	-1.674856	0.304953
H	-3.747423	-0.947031	0.089278
C	2.060146	-0.360715	0.060572
C	3.311857	-0.103466	0.026929
C	-0.806961	1.466646	-0.359042

Vibrational frequencies

-195.4585	47.1451	124.8440
-----------	---------	----------

225.9415	236.6285	290.1310
376.5589	431.9862	543.2743
547.9161	791.7605	820.6371
891.2228	938.8304	1164.3967
1406.2800	1797.3102	2038.9499
2072.4454	3164.3003	3462.1020

i2 – i3

Cartesian coordinates

C	-0.427529	0.170820	-0.653848
C	-1.627768	-0.128684	0.062295
C	-2.646842	-0.361183	0.653348
C	0.823425	-0.621010	-0.491332
H	0.985383	-1.419045	-1.214583
H	-3.542653	-0.572546	1.187299
C	1.691250	-0.395958	0.476782
C	2.544774	-0.194322	1.414789
C	-0.653698	1.205175	-1.434818

Vibrational frequencies

-145.9671	83.0975	140.0590
181.2089	213.4947	266.8048
410.3727	436.7778	605.3626
665.3062	771.0504	804.9755
883.4059	1113.2486	1205.2113
1379.4190	1693.1780	2068.4316
2227.9688	3157.6705	3481.1680

i4 – i17

Cartesian coordinates

C	0.633994	-0.767302	-0.005126
C	1.737326	0.503475	-0.005943
C	1.672100	1.715344	-0.001890
C	-0.767541	-0.766693	0.000968
H	-1.210398	-1.763590	-0.000227
H	1.598416	2.777376	0.001739
C	-1.521474	0.334980	0.007691
C	-2.219809	1.402871	0.014060
C	1.901217	-0.976334	-0.011291

Vibrational frequencies

-251.4126	92.3541	124.1132
220.7780	261.9436	307.8133
360.8438	430.3839	620.4663
632.1145	718.9024	839.6745
871.2342	932.1518	1141.7639
1384.9029	1829.7954	2060.0915
2095.0328	3139.5089	3470.4562

i15 – i17

Cartesian coordinates

C	1.010341	0.142914	0.000231
C	2.339428	-0.111618	-0.000016
C	3.525142	-0.337553	-0.000148
C	-4.005045	0.041732	-0.004062
H	4.570018	-0.539564	-0.000276
C	-2.719720	0.122037	-0.003104
C	-1.493398	0.692759	0.001598
C	-0.201993	0.332595	0.000261
H	-2.752409	1.364645	0.005760

Vibrational frequencies

-1846.4721	5.2295	77.9026
139.0701	183.9440	291.3087
311.5594	342.4026	452.7638
497.0379	585.2122	619.9476
624.6590	768.6320	1061.0491
1472.2900	1809.0863	2111.3885
2221.1229	2374.6084	3475.2727

iI – i7

Cartesian coordinates

C	0.217532	-0.455745	-0.005988
C	1.544642	-0.090682	-0.010293
C	2.681052	0.307740	-0.016332
C	-0.683554	-1.406878	0.016445
H	-0.786796	-2.481989	0.045847
H	3.689044	0.649489	-0.021370
C	-1.592046	-0.317073	-0.017599
C	-2.389109	0.762666	-0.051247
C	-1.063076	1.202749	-0.057776

Vibrational frequencies

-424.8732	109.7443	133.9871
245.1128	344.4068	436.9280
532.2593	547.6988	646.5276
650.2622	746.5046	817.0448
875.0852	936.8693	1143.2230
1238.8355	1707.7061	1781.3358
2223.2646	3240.7748	3475.7513

i0 – iI

Cartesian coordinates

C	-1.188122	-1.192466	0.449375
C	-0.677531	0.077924	0.228240
C	-0.680286	1.298327	0.136019
C	-1.631856	-2.289441	0.640958
H	-2.027898	-3.262287	0.811468
H	-0.543198	2.348693	0.022640
C	1.228692	-0.038107	-0.227714
C	2.018174	0.968420	-0.497682
C	3.043052	1.673848	-0.803054

Vibrational frequencies

-441.9817	41.8344	106.1663
182.4328	191.7984	249.3124
249.8686	418.2842	499.0572
537.9117	664.8948	714.3673
721.6078	739.4126	905.3903
1265.8784	2057.6715	2074.9554
2304.4256	3466.4484	3480.6348

i7 – i8

Cartesian coordinates

C	0.118544	-0.021006	0.350995
C	1.497258	0.093278	0.098131
C	2.682770	0.180018	-0.078084
C	-0.782416	-1.098037	0.132029
H	-0.618182	-2.153374	-0.010386
H	3.731337	0.261133	-0.240301
C	-1.723584	-0.203777	-0.386210
C	-2.108474	1.162234	0.029533
C	-0.857767	1.026213	0.332889

Vibrational frequencies

-225.9150	134.4567	180.3408
350.6041	506.4939	519.3105
603.5588	669.1704	671.1638
711.2115	740.0895	763.1366
861.2980	1028.7255	1139.8453
1336.6485	1400.9842	1723.6028
2234.3016	3285.7850	3478.7110

i6 – i7**Cartesian coordinates**

C	0.158800	-0.447374	0.286582
C	1.533269	-0.561774	-0.037041
C	2.709618	-0.665198	-0.250064
C	-0.847406	-1.425734	0.336001
H	-0.860336	-2.488174	0.522588
H	3.751403	-0.754963	-0.449930
C	-1.548228	-0.586406	-0.527519
C	-1.595176	1.537598	-0.218651
C	-0.671791	0.682886	0.031264

Vibrational frequencies

-253.2695	141.4328	170.1443
259.3111	368.6262	520.2101
540.8733	626.8467	711.9589
738.2621	769.9797	795.3640
804.4391	1072.4513	1137.8573
1323.9953	1445.4206	1924.0600
2245.5786	3275.0776	3476.8246

i12 – i14**Cartesian coordinates**

C	0.704414	0.435895	0.000012
C	1.395455	-0.728793	0.000037
C	1.102245	-1.946201	0.000063
C	0.000566	1.654152	-0.000014
H	-1.464709	-2.956142	0.000085
H	1.455377	-2.959455	0.000085
C	-0.706045	0.437496	0.000012
C	-1.399728	-0.725621	0.000037
C	-1.109281	-1.943692	0.000063

Vibrational frequencies

-453.6451	209.4821	318.0094
437.5240	510.9083	524.6914
547.1934	633.4817	705.4177
744.2938	769.3243	777.4837
856.6789	963.6569	1068.4740
1415.3274	1648.3574	1894.4858
1964.7053	3365.5393	3365.5602

i12 – i13**Cartesian coordinates**

C	1.026537	0.462101	-0.529344
C	1.274510	-0.800412	-0.428733
C	0.739947	-1.914605	0.094881
C	0.000208	1.038700	0.000808
H	-1.287719	-2.634282	-0.697661
H	1.278579	-2.638370	0.696221
C	-1.027516	0.464392	0.530823
C	-1.278986	-0.797355	0.428920
C	-0.747265	-1.912531	-0.095536

Vibrational frequencies

-474.6895	243.9192	349.3776
356.1580	452.9368	456.5386
526.4164	556.8511	763.6682
770.5187	1042.7575	1127.0613
1153.4873	1287.7909	1354.3453
1468.6462	1669.2454	1791.5321
1921.0026	3179.0606	3182.1863

i2 – i4**Cartesian coordinates**

C	-0.585891	-0.781672	0.000000
C	-1.267494	0.511744	0.000000
C	-1.568451	1.685539	0.000000
C	0.814797	-1.082269	0.000000
H	1.056708	-2.143234	0.000000
H	-1.842499	2.714900	0.000000
C	1.768218	-0.154333	0.000000
C	2.666871	0.753528	0.000000
C	-1.841127	-1.147574	0.000000

Vibrational frequencies

-43.4181	100.7110	131.7681
250.3921	265.4550	280.4699
366.2118	478.1488	573.2636
593.3836	768.7895	832.4252
908.7069	1050.8077	1173.2194
1391.9381	1775.2413	2062.3934
2100.3163	3170.8466	3466.3242

i8 – i15**Cartesian coordinates**

C	0.407530	0.286797	0.689306
C	1.681182	0.214549	0.227895
C	2.856075	0.137861	-0.074473
C	-1.229058	-1.729581	0.261838
H	-0.688699	-2.446034	-0.350024
H	3.879296	0.077474	-0.361529
C	-1.696023	-0.584193	-0.183742
C	-2.033673	0.758677	-0.348665
C	-0.751064	0.533892	0.040655

Vibrational frequencies

-129.9468	76.4374	143.5506
263.6466	370.5875	441.0991
459.2846	481.4403	508.3795
573.0638	724.0475	769.5606
858.0237	941.0427	983.0307
1271.4360	1374.2317	1855.6859
2100.9862	3217.1006	3471.8358

i3 – i5**Cartesian coordinates**

C	0.446649	0.255677	-0.150804
C	1.834981	0.062813	0.020741
C	3.010521	-0.103154	0.187184
C	-0.610557	-0.721394	-0.294055
H	-0.404207	-1.670448	-0.787927
H	4.054682	-0.245987	0.334928
C	-1.856967	-0.306402	0.004891
C	-2.994493	0.019999	0.493005

C	-0.266298	1.305481	-0.587573
---	-----------	----------	-----------

Vibrational frequencies

-227.2893	95.0470	138.7263
193.4081	245.0106	329.0961
453.3241	497.6814	539.3144
722.3858	755.7969	865.1438
895.5361	1105.7613	1219.8584
1316.4647	1633.7174	2021.1963
2262.4839	3151.1003	3479.1339

i1 – i9

Cartesian coordinates

C	-1.239676	-0.809323	0.283401
C	-0.956708	0.512323	0.374666
C	-0.618890	1.806505	0.444708
C	-0.485208	-1.753839	-0.086270
H	-0.392446	-2.808370	-0.260459
H	-0.939495	2.810039	0.684407
C	0.418479	1.021878	0.006944
C	1.329661	0.158868	-0.401417
C	1.488943	-1.092731	-0.623810

Vibrational frequencies

-379.3209	165.6995	293.0098
382.7011	484.5604	486.1878
560.0278	592.3466	641.8666
777.7500	816.8793	837.5483
884.0320	1010.6042	1109.0523
1554.6015	1727.6283	1891.9149
1908.0243	3256.6602	3370.8217

i1 – i2

Cartesian coordinates

C	-0.505938	0.656870	-0.000002
C	-1.643167	-0.162207	-0.000001
C	-2.602826	-0.879396	0.000000
C	-0.164005	1.961848	-0.000003
H	1.310819	1.553130	-0.000003
H	-3.453497	-1.519495	0.000000
C	0.887191	0.461891	-0.000001
C	1.791127	-0.513014	0.000000
C	2.672832	-1.428119	0.000000

Vibrational frequencies

-325.7057	120.7666	150.1557
211.0629	216.6220	343.9713
442.3359	542.0696	660.4634
699.9642	735.2813	754.9901
883.9127	1013.7465	1099.1693
1514.5459	1692.7455	2071.6134
2274.4495	2513.7207	3478.9768

i17 – i18

Cartesian coordinates

C	-1.996359	-1.279087	0.024435
C	-2.813200	-0.191113	0.018136
C	-3.623383	0.714172	0.017988
C	2.998919	-2.551000	-0.124138
C	1.788279	-2.161204	-0.090985
C	0.543460	-1.786976	-0.055953
C	-0.674895	-1.347888	-0.024194

H	-4.333131	1.506987	0.017688
H	0.166675	-0.413286	-0.089179

Vibrational frequencies

-1032.8834	84.9565	97.4437
170.7025	202.6720	313.6659
374.6506	468.1097	497.5459
559.0835	634.2202	677.6998
824.7392	868.8195	1061.5227
1474.8686	1877.0266	2084.8363
2162.7987	2200.0768	3474.7977

i10 – i12

Cartesian coordinates

C	0.112935	1.331501	-0.081628
C	1.362764	0.845080	0.004818
C	1.524859	-0.649472	0.126199
C	-1.036670	0.650588	-0.074076
C	-2.128725	-0.196965	-0.051129
C	-0.867670	-0.821852	0.045540
C	0.353344	-1.293268	0.129504
H	1.095678	2.168465	-0.106499
H	2.517825	-1.070160	0.198122

Vibrational frequencies

-1748.2687	169.8450	371.5653
451.7438	485.5053	538.4189
605.7888	617.9909	668.6033
671.7405	772.7333	874.8985
887.1880	1016.4403	1217.2658
1371.0149	1437.3491	1678.8121
1783.3843	2239.1084	3259.3085

i10 – i11

Cartesian coordinates

C	-1.366256	0.228475	0.002354
C	-0.113560	0.795296	0.000760
C	1.052175	0.019300	-0.000410
C	-1.402628	-1.400056	0.002786
C	-0.182083	-1.760055	0.001453
C	1.082363	-1.409486	-0.000102
C	2.284856	-0.616385	-0.001691
H	-0.043807	1.877114	0.000420
H	-2.377413	-0.641528	0.003741

Vibrational frequencies

-1766.9606	219.6803	267.7247
339.2642	486.7859	500.7254
564.0538	601.4085	647.4076
737.2518	805.4133	846.9950
980.5050	1028.3929	1159.1439
1391.3144	1419.7025	1626.2066
1864.2598	2361.5570	3217.6173

i1 – i5

Cartesian coordinates

C	-0.002098	0.035390	0.336109
C	-0.087631	-0.670875	-0.866640
C	-0.177444	-1.276730	-1.897428
C	0.174730	0.011270	1.626220
H	-0.257166	-1.814207	-2.812912
H	0.623730	-0.358254	2.529533

C	-0.793344	2.358300	2.994384
C	-0.219749	1.903864	1.940488
C	0.210043	1.400705	0.746176

Vibrational frequencies

-624.6937	102.6604	161.3401
232.2776	270.9398	399.7897
470.8013	515.7269	550.1200
615.9727	727.0864	761.8251
774.6837	910.7171	992.7132
1166.4986	1776.0969	1849.2223
2267.2817	3332.6630	3478.9100

Products

p1 (l-C7H)

Cartesian coordinates

C	1.236554	-0.057888	-0.000002
C	2.583199	-0.109590	-0.000002
C	3.791430	-0.155977	-0.000001
C	-3.874386	0.137427	0.000000
H	4.855251	-0.196847	-0.000002
C	-2.574763	0.087825	0.000000
C	-1.305989	0.039503	0.000000
C	0.004170	-0.010692	-0.000001

Vibrational frequencies

76.2865	170.4009	184.8500
297.5352	326.3503	404.4333
546.2951	552.5836	564.1355
615.1024	702.8557	759.3791
1080.0407	1572.5182	1878.7412
2098.4579	2196.3676	3471.0971