New light on the imbroglio surrounding the $C_8H_6^+$ isomers formed from ionized azulene and naphthalene using ion-molecule reactions

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1 Chemicals

PA (98% purity), **Naph** (99% purity), and **Azu** (99% purity) were purchased from Sigma-Aldrich. Propyne (99% purity) and allene (96% purity) were purchased from ABCR GMBH – Germany. All samples were used without further purification.

2 Cross section determination

Reaction cross sections are derived from the Beer-Lambert law.

As detailed in Cunha de Miranda et al. [2015], when reactant ions pass the scattering cell, the infinitesimal increase of product ions is:

$$\mathrm{d}I_{\mathrm{pro}} = -\mathrm{d}I_{\mathrm{par}} = I_{\mathrm{par}}(x) \cdot n\sigma \cdot \mathrm{d}x, \tag{1}$$

where I_{pro} are the product ions, I_{par} the parent ions and n is the neutral density in the scattering cell. Integration along the length l_{Cell} of the scattering cell yields to:

$$I_{\mathrm{par}}(l_{\mathrm{Cell}}) = I_0 \cdot \exp(-n \cdot \sigma \cdot l_{\mathrm{Cell}}) \Leftrightarrow \sigma = -\frac{1}{n \cdot l_{\mathrm{Cell}}} \cdot \ln\left(\frac{I_{\mathrm{par}}(l_{\mathrm{Cell}})}{I_0}\right) \tag{2}$$

with I_0 being the parent ion intensity at the entrance of the scattering cell. As $I_{\mathrm{par}} = I_0 - I_{\mathrm{pro}}$, we have

$$\sigma = -\frac{1}{n \cdot l_{\mathrm{Cell}}} \cdot \ln\left(\frac{I_0 - I_{\mathrm{pro}}}{I_0}\right) = -\frac{1}{n \cdot l_{\mathrm{Cell}}} \cdot \ln\left(1 - \frac{I_{\mathrm{pro}}}{I_0}\right) \tag{3}$$

If $I_{\mathrm{pro}} \ll I_0$ (less than 10%), σ can be approximated using $\ln(1-x) = -x$ for $x \ll 1$, leading to

$$\sigma = \frac{1}{n \cdot l_{\mathrm{Cell}}} \cdot \frac{I_{\mathrm{pro}}}{I_0} \tag{4}$$

As the scattering cell is an open device, pressure is not completely uniform inside. Also, reactions are possible with the diffused gas molecules outside the scattering cell. It is therefore appropriate to replace l_{Cell} by an effective length l_{eff} and to determine its value by a calibration. Like many other groups, we use the results of Ervin and Armentrout [1985] for the reaction $\mathrm{Ar}^+ + \mathrm{D}_2 \rightarrow \mathrm{ArD}^+ + \mathrm{D}$. The kinematics of this reaction ensures that no calibration uncertainties arise from different masses or velocities of products and parents. We finally obtain

$$\sigma = \frac{9.14 \times 10^4}{P(\text{in nbar})} \cdot \frac{I_{\mathrm{pro}}}{I_0} \tag{5}$$

where the pressure P is measured with a differential baratron (MKS 398H digital manometer). Neutral gas is supplied at maximum pressures of 100 nbar. We take care to ensure single collision conditions, which in practice means that attenuation of the parent ion beam should be smaller than 10%.

In order to correct for reactions occurring outside of the cell by interaction of parent ions with the diffused gas, two measurements are systematically performed with the same flux of neutral gas sent either in the cell or in the chamber containing the cell. By this, we derive two values of sigma, σ_{cell}, which represents reactions occurring in the cell and in the diffusion path to the pump and $\sigma_{\mathrm{chamber}}$,which represents only the reactions occurring on the diffusion path to the pump. The difference between the two values $\sigma_{\mathrm{cell}} - \sigma_{\mathrm{chamber}}$ is the final value of cross section, tabulated in the present study.

3 Supplementary Figures

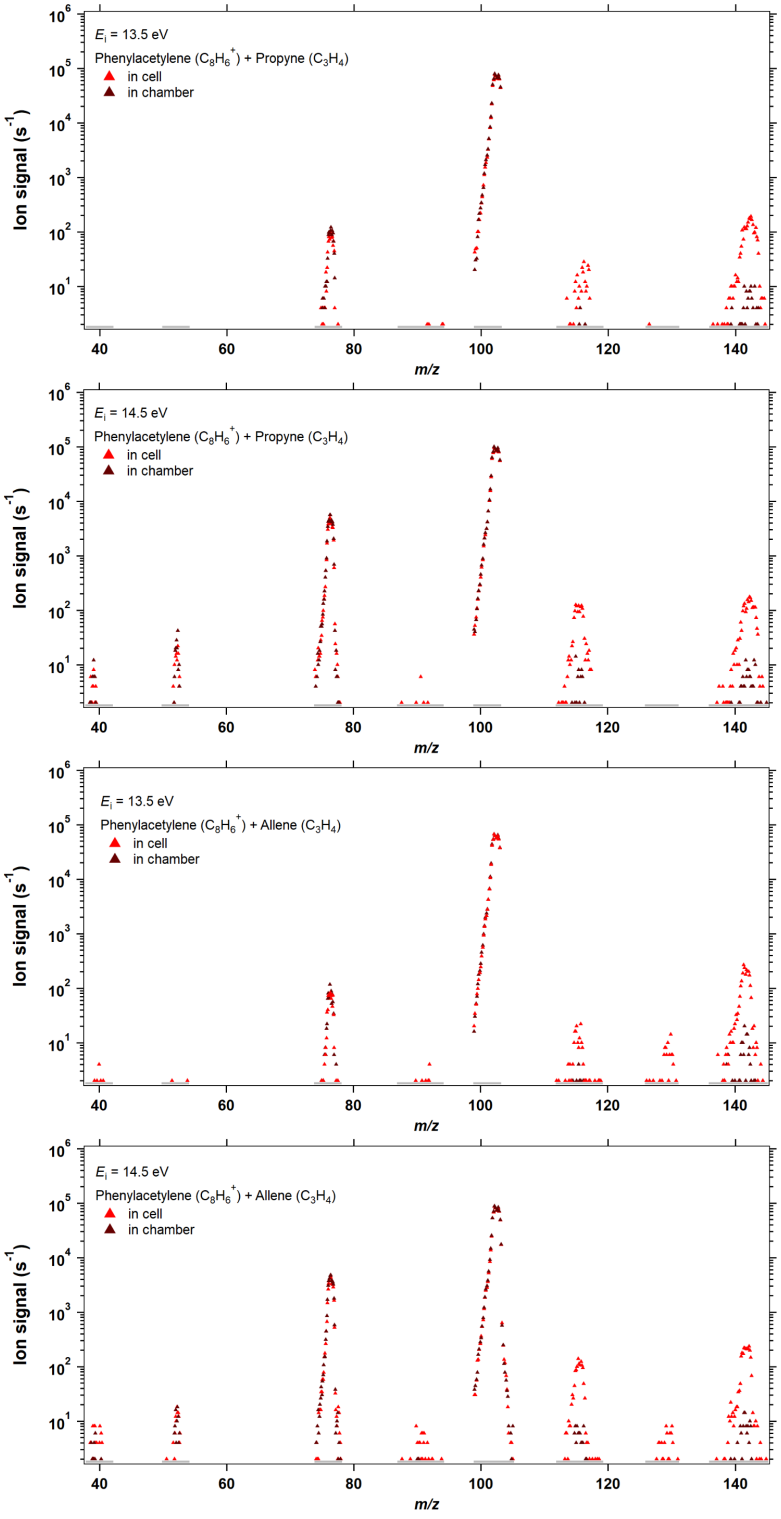

Figure S1: Mass spectra of $C_8H_6^+$ generated by photoionization of **PA** at two different photon energies, reacting with Propyne (top panels) and Allene (bottom panels). The mass range was scanned in differents segments, indicated by the gray bars on the x-axis.

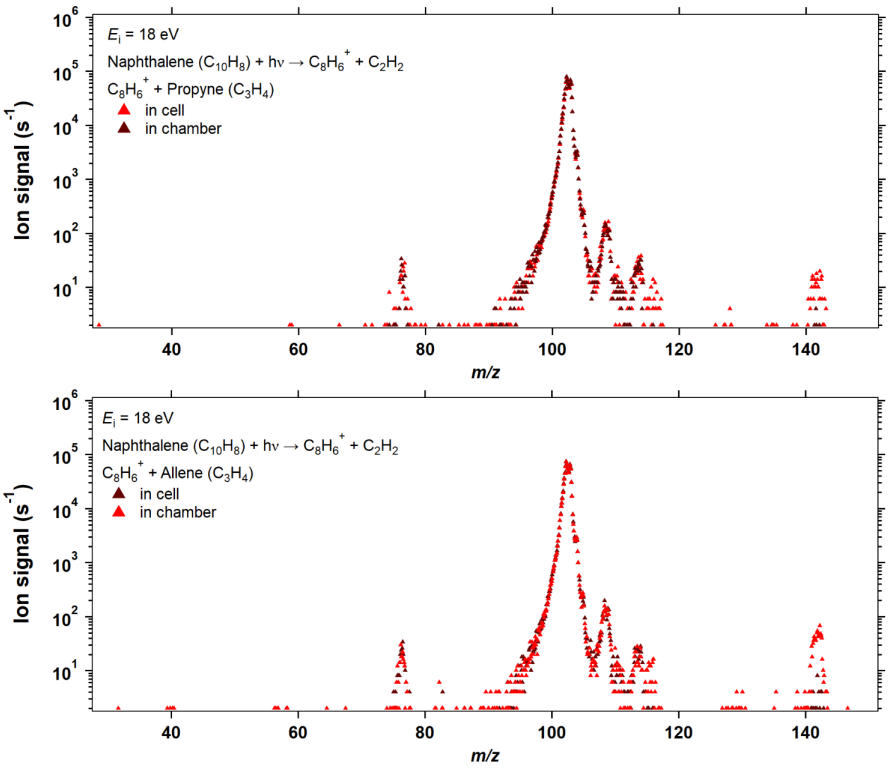

Figure S2: Mass spectra of $C_8H_6^+$ generated by dissociative ionization of Naphthalene at a photon energy of 18 eV, reacting with Propyne (top panel) and Allene (bottom panel).

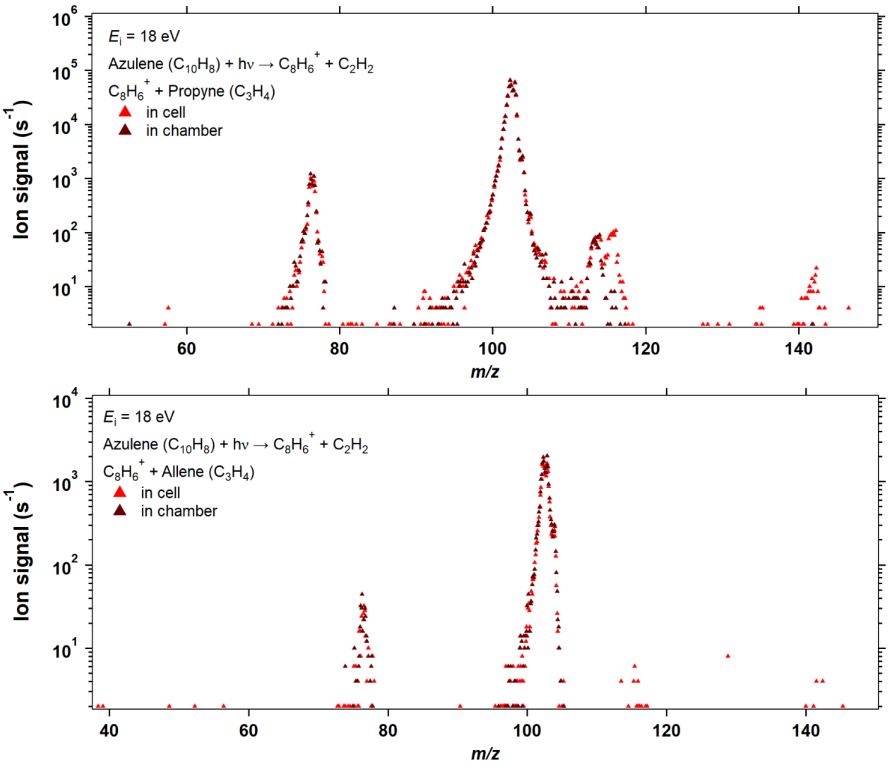

Figure S3: Mass spectra of $C_8H_6^+$ generated by dissociative ionization of Azulene at a photon energy of 18 eV, reacting with Propyne (top panel) and Allene (bottom panel).

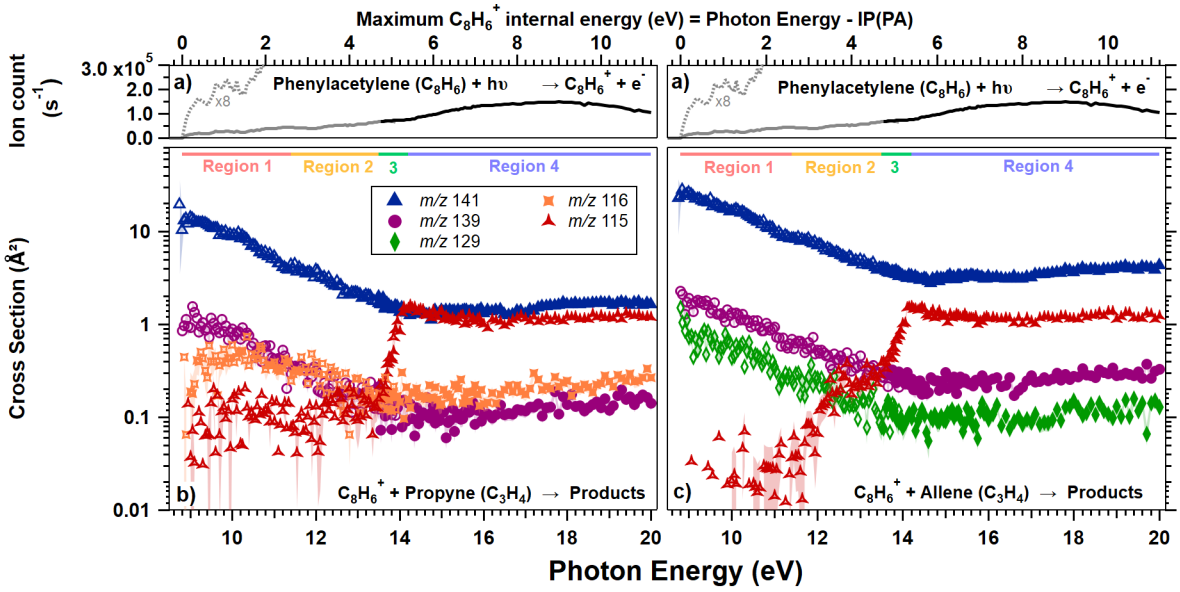

Figure S4: The top panels (black traces) display the $C_8H_6^+$ photoion yield starting from phenylacetylene precursor (gray region was recorded with Kr in gas filter while dark region was recorded with Ne in gas filter). Bottom panels are reaction cross sections for the products resulting from $C_8H_6^+$ produced from phenyacetylene reacting, from left to right, with propyne and allene as a function of photon energy. The error bars are given in shaded colors in bottom panels.

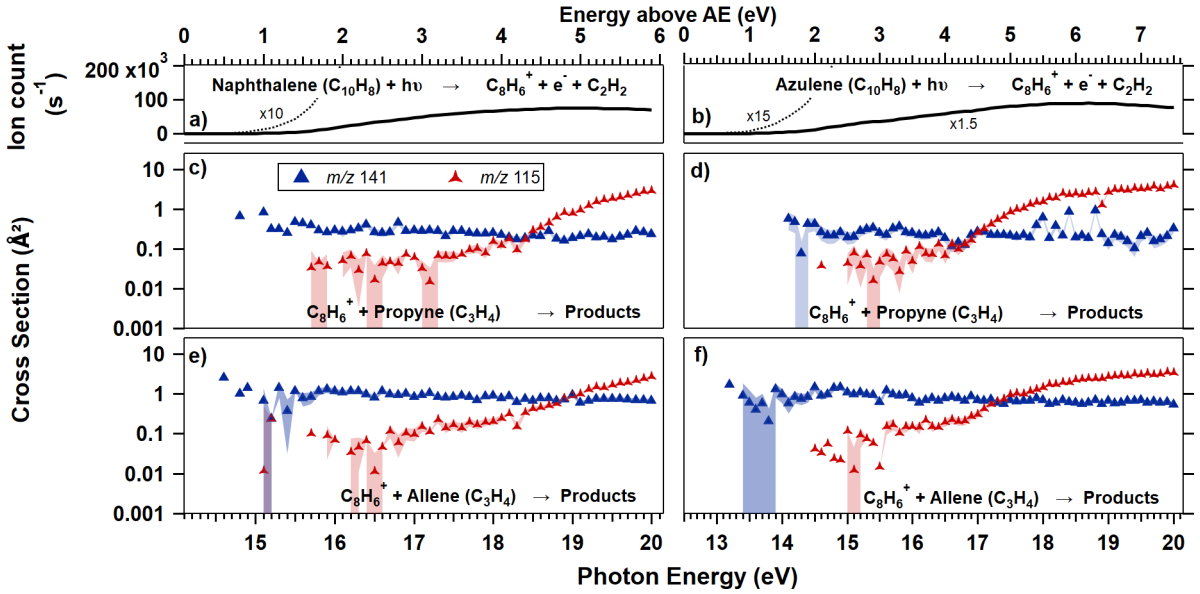

Figure S5: The top panels (black traces), a) and b), display the $C_8H_6^+$ photoion yield starting from **Naph** and **Azu** precursors, respectively. Middle panels, c) and d), are reaction cross sections of $C_8H_6^+$ with propyne as a function of photon energy starting with **Naph** and **Azu** as precursors, respectively. Bottom panels, e) and f), are the reaction cross sections with allene from **Naph** and from **Azu**), respectively. We defined the AE as the energy of the photon where more than 20 $C_8H_6^+$ ions/s are detected. The error bars are given in shaded colors in bottom panels.

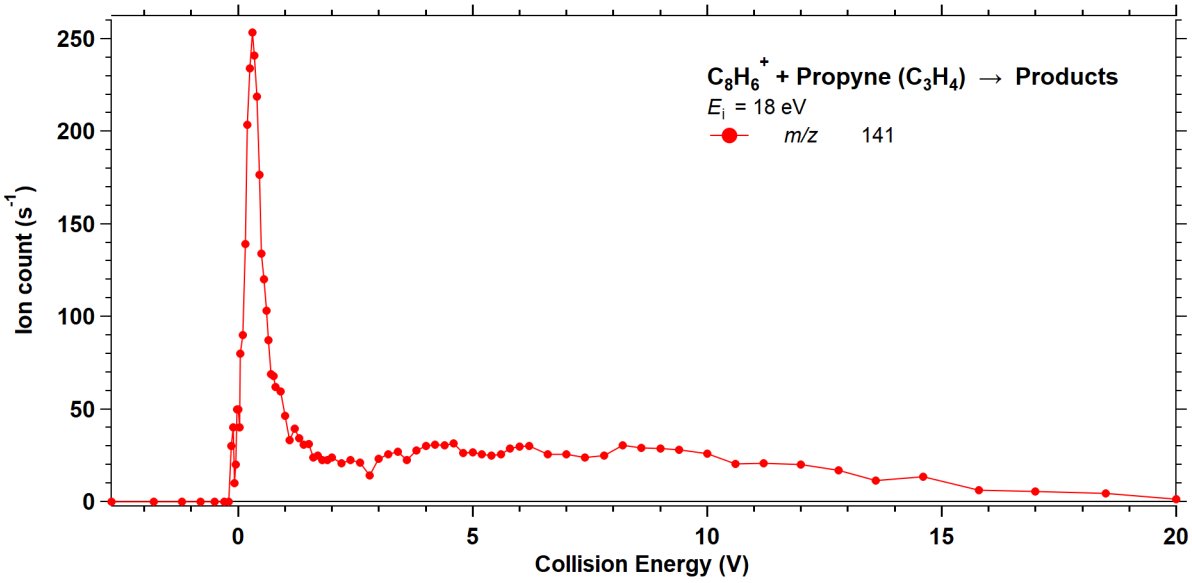

Figure S6: Reaction cross section of $C_8H_6{}^+$–generated from **PA** at photon energy of 18 eV– with propyne as a function collision energy.

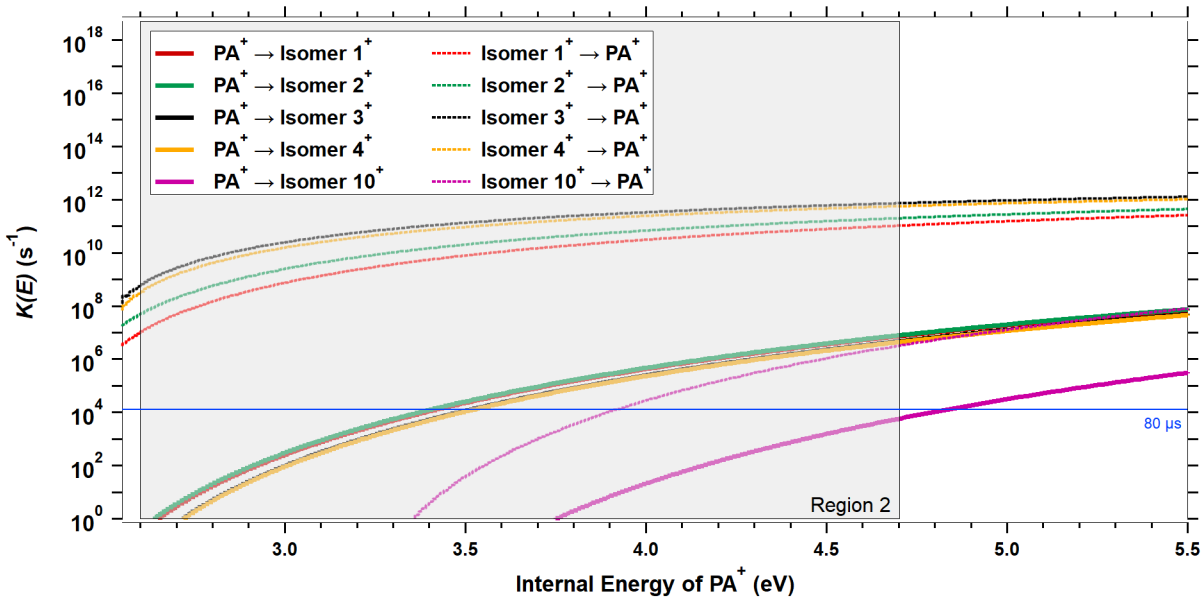

Figure S7: Microcanonical rate constants for interconversion from $\mathbf{PA}^+$ to $\mathbf{1}^+$, $\mathbf{2}^+$, $\mathbf{3}^+$, $\mathbf{4}^+$, and $\mathbf{10}^+$ (solid lines) and the corresponding back reactions (dashed lines) as a function of the internal energy of $\mathbf{PA}^+$. The shaded grey area represents the energies accessible in region 2.

4 Supplementary Tables

Table S1: Reaction products for $C_8H_6^+$ from **PA** reacting with **Propyne** and **Allene**.

Reactant	Product	*m/z*	Mechanism
Propyne	$C_{11}H_9^+$	141	Adduct formation followed by loss of H
Propyne	$C_{11}H_7^+$	139	Adduct formation followed by loss of H and H_2
Propyne	$C_9H_8^+$	116	Adduct formation followed by loss of C_2H_2
Propyne	$C_9H_7^+$	115	Adduct formation followed by loss of CH_2CH
Allene	$C_{11}H_9^+$	141	Adduct formation followed by loss of H
Allene	$C_{11}H_7^+$	139	Adduct formation followed by loss of H and H_2
Allene	$C_{10}H_9^+$	129	Adduct formation followed by loss of CH
Allene	$C_9H_7^+$	115	Adduct formation followed by loss of CH_2CH

Table S2: Reaction products for $C_8H_6^+$ from **Naph** and **Azu** reacting with **Propyne** and **Allene**.

Reactant	Product	*m/z*	Mechanism
Propyne	$C_{11}H_9^+$	141	Adduct formation followed by loss of H
Propyne	$C_9H_7^+$	115	Adduct formation followed by loss of CH_2CH
Allene	$C_{11}H_9^+$	141	Adduct formation followed by loss of H
Allene	$C_9H_7^+$	115	Adduct formation followed by loss of CH_2CH

Table S3: Reaction cross sections to form m/z 115 from $C_8H_6^+$ generated from **PA** reacting with allene. Kr in the gas filter.

Energy/eV	Sigma/A²	Energy/eV	Sigma/A²	Energy/eV	Sigma/A²
8.7000000	0.0000000	10.450000	0.0000000	12.200000	0.1446714
8.7500000	0.0000000	10.500000	0.0191286	12.250000	0.1612194
8.8000000	0.0000000	10.550000	0.0178393	12.300000	0.2567257
8.8500000	0.0000000	10.600000	0.0156125	12.350000	0.1787439
8.9000000	0.0000000	10.650000	0.0173836	12.400000	0.1113478
8.9500000	0.0000000	10.700000	0.0000000	12.450000	0.1864153
9.0000000	0.0000000	10.750000	0.0297057	12.500000	0.3197050
9.0500000	0.0335949	10.800000	0.0283938	12.550000	0.1991233
9.1000000	0.0000000	10.850000	0.0278642	12.600000	0.2705186
9.1500000	0.0000000	10.900000	0.0278315	12.650000	0.2690573
9.2000000	0.0000000	10.950000	0.0281211	12.700000	0.3775088
9.2500000	0.0000000	11.000000	0.0141332	12.750000	0.2295561
9.3000000	0.0000000	11.050000	0.0273999	12.800000	0.1780339
9.3500000	0.0000000	11.100000	0.0399555	12.850000	0.2078794
9.4000000	0.0000000	11.150000	0.0517331	12.900000	0.2450375
9.4500000	0.0289384	11.200000	0.0000000	12.950000	0.2233284
9.5000000	0.0000000	11.250000	0.0121998	13.000000	0.2095857
9.5500000	0.0235289	11.300000	0.0000000	13.050000	0.2346857
9.6000000	0.0000000	11.350000	0.0243578	13.100000	0.2513954
9.6500000	0.0000000	11.400000	0.0367975	13.150000	0.3669185
9.7000000	0.0608640	11.450000	0.0623856	13.200000	0.2156623
9.7500000	0.0000000	11.500000	0.0378224	13.250000	0.2676259
9.8000000	0.0000000	11.550000	0.0387844	13.300000	0.3134666
9.8500000	0.0000000	11.600000	0.0258345	13.350000	0.2755503
9.9000000	0.0188347	11.650000	0.0130752	13.400000	0.2329896
9.9500000	0.0000000	11.700000	0.0530903	13.450000	0.2898250
10.000000	0.0207782	11.750000	0.0820247	13.500000	0.3836992
10.050000	0.0241342	11.800000	0.0826616	13.550000	0.3917061
10.100000	0.0190817	11.850000	0.0822754	13.600000	0.3363986
10.150000	0.0000000	11.900000	0.0682870	13.650000	0.4290393
10.200000	0.0000000	11.950000	0.0409793	13.700000	0.4669811
10.250000	0.0460816	12.000000	0.0667713	13.750000	0.4303103
10.300000	0.0709973	12.050000	0.1187894	13.800000	0.5522698
10.350000	0.0000000	12.100000	0.1302878	13.850000	0.6697499
10.400000	0.0189924	12.150000	0.1366482	13.900000	0.7528005

Table S4: Reaction cross sections to form m/z 115 from $C_8H_6^+$ generated from **PA** reacting with allene. Ne in the gas filter.

Energy/eV	Sigma/A²	Energy/eV	Sigma/A²	Energy/eV	Sigma/A²
13.5500000	0.3232834	15.0500000	1.0502326	17.1000000	1.0176324
13.6000000	0.3557838	15.1000000	1.2941538	17.2000000	1.1652565
13.6500000	0.3707547	15.1500000	1.1742060	17.3000000	1.2076330
13.7000000	0.4556333	15.2000000	1.2122545	17.4000000	1.2100731
13.7500000	0.5556046	15.2500000	1.2970597	17.5000000	1.1765767
13.8000000	0.4982941	15.3000000	1.2521408	17.6000000	1.1268605
13.8500000	0.7019489	15.3500000	1.1952136	17.7000000	1.2304184
13.9000000	0.7805923	15.4000000	1.2047486	17.8000000	1.2252383
13.9500000	0.8671439	15.4500000	1.2853589	17.9000000	1.1596589
14.0000000	1.0088753	15.5000000	1.1929883	18.0000000	1.1597970
14.0500000	1.0396519	15.5500000	1.1716189	18.1000000	1.1403750
14.1000000	1.5100945	15.6000000	1.1720849	18.2000000	1.2934397
14.1500000	1.5455704	15.6500000	1.1563933	18.3000000	1.1984068
14.2000000	1.5690864	15.7000000	1.2180020	18.4000000	1.2537371
14.2500000	1.4675868	15.7500000	0.9929348	18.5000000	1.2388856
14.3000000	1.4739594	15.8000000	1.0882964	18.6000000	1.3235241
14.3500000	1.4284836	15.8500000	1.0623102	18.7000000	1.2383780
14.4000000	1.4602454	15.9000000	1.1666179	18.8000000	1.3657962
14.4500000	1.5419936	15.9500000	1.2068177	18.9000000	1.3679274
14.5000000	1.4600999	16.0000000	1.1469276	19.0000000	1.1272619
14.5500000	1.2675064	16.1000000	1.1946595	19.1000000	1.2147735
14.6000000	1.2061712	16.2000000	1.1489625	19.2000000	1.3303977
14.6500000	1.3169668	16.3000000	1.1261550	19.3000000	1.3259546
14.7000000	1.4078137	16.4000000	1.1798788	19.4000000	1.1808822
14.7500000	1.1662393	16.5000000	1.1596699	19.5000000	1.1739740
14.8000000	1.2862867	16.6000000	1.0246606	19.6000000	1.1544542
14.8500000	1.3884503	16.7000000	1.1784751	19.7000000	1.3249918
14.9000000	1.2152473	16.8000000	1.0111654	19.8000000	1.2795647
14.9500000	1.2263316	16.9000000	1.1728152	19.9000000	1.1370683
15.0000000	1.2153089	17.0000000	1.0810577	20.0000000	1.2249573

Table S5: Reaction cross sections to form m/z 115 from $C_8H_6^+$ generated from **Naph** reacting with allene.

Energy/eV	Sigma/A²	Energy/eV	Sigma/A²	Energy/eV	Sigma/A²
12.5000000	0.0000000	15.1000000	0.0117042	17.7000000	0.1938995
12.6000000	0.0000000	15.2000000	0.2412967	17.8000000	0.1688577
12.7000000	0.0000000	15.3000000	0.0000000	17.9000000	0.1963217
12.8000000	0.0000000	15.4000000	0.0000000	18.0000000	0.2054619
12.9000000	0.0000000	15.5000000	0.0000000	18.1000000	0.2444474
13.0000000	0.0000000	15.6000000	0.0000000	18.2000000	0.3164135
13.1000000	NAN	15.7000000	0.1031534	18.3000000	0.1537099
13.2000000	0.0000000	15.8000000	NAN	18.4000000	0.3442089
13.3000000	0.0000000	15.9000000	0.0904572	18.5000000	0.4349679
13.4000000	NAN	16.0000000	0.0710028	18.6000000	0.4543165
13.5000000	0.0000000	16.1000000	NAN	18.7000000	0.5179300
13.6000000	0.0000000	16.2000000	0.0342596	18.8000000	0.5839139
13.7000000	0.0000000	16.3000000	0.0459002	18.9000000	0.7702425
13.8000000	0.0000000	16.4000000	0.0684424	19.0000000	0.9068183
13.9000000	0.0000000	16.5000000	0.0115635	19.1000000	0.9874797
14.0000000	0.0000000	16.6000000	0.0459016	19.2000000	1.3087095
14.1000000	NAN	16.7000000	0.1184502	19.3000000	1.5174700
14.2000000	0.0000000	16.8000000	0.0603995	19.4000000	1.4379933
14.3000000	0.0000000	16.9000000	0.1040801	19.5000000	1.6533824
14.4000000	0.0000000	17.0000000	0.0989635	19.6000000	1.8857253
14.5000000	NAN	17.1000000	0.1528001	19.7000000	1.9655797
14.6000000	0.0000000	17.2000000	0.1114948	19.8000000	2.1453702
14.7000000	0.0000000	17.3000000	0.2301905	19.9000000	2.4675455
14.8000000	0.0000000	17.4000000	0.1418415	20.0000000	2.6860280
14.9000000	0.0000000	17.5000000	0.1713146		
15.0000000	NAN	17.6000000	0.1439517		

Table S6: Reaction cross sections to form m/z 115 from $C_8H_6^+$ generated from **Azu** reacting with allene.

Energy/eV	Sigma/A^2	Energy/eV	Sigma/A^2	Energy/eV	Sigma/A^2
12.0000000	0.0000000	14.7000000	0.0568583	17.4000000	0.7556168
12.1000000	0.0000000	14.8000000	0.0241876	17.5000000	0.9501532
12.2000000	0.0000000	14.9000000	0.0225326	17.6000000	1.0436096
12.3000000	0.0000000	15.0000000	0.1172010	17.7000000	1.0108134
12.4000000	0.0000000	15.1000000	0.0121369	17.8000000	1.1789734
12.5000000	0.0000000	15.2000000	0.0928325	17.9000000	1.3189744
12.6000000	0.0000000	15.3000000	0.0763540	18.0000000	1.4496131
12.7000000	0.0000000	15.4000000	0.0583136	18.1000000	1.7189652
12.8000000	NAN	15.5000000	0.0146244	18.2000000	1.7337790
12.9000000	0.0000000	15.6000000	0.1512502	18.3000000	1.9512336
13.0000000	0.0000000	15.7000000	0.1731345	18.4000000	1.9319919
13.1000000	0.0000000	15.8000000	0.1061001	18.5000000	2.2615030
13.2000000	0.0000000	15.9000000	0.1533903	18.6000000	2.3335321
13.3000000	0.0000000	16.0000000	0.1499277	18.7000000	2.4583378
13.4000000	0.0000000	16.1000000	0.1447004	18.8000000	2.4346204
13.5000000	0.0000000	16.2000000	0.2222510	18.9000000	2.4225318
13.6000000	0.0000000	16.3000000	0.1530709	19.0000000	2.7380869
13.7000000	0.0000000	16.4000000	0.1448781	19.1000000	2.7895994
13.8000000	0.0000000	16.5000000	0.1959212	19.2000000	2.9195783
13.9000000	0.0000000	16.6000000	0.2264925	19.3000000	2.8497479
14.0000000	0.0000000	16.7000000	0.2030744	19.4000000	3.1516025
14.1000000	0.0000000	16.8000000	0.2101669	19.5000000	3.0869572
14.2000000	0.0000000	16.9000000	0.2759400	19.6000000	3.3262012
14.3000000	0.0000000	17.0000000	0.3023333	19.7000000	2.9884281
14.4000000	0.0000000	17.1000000	0.4367716	19.8000000	3.1845527
14.5000000	0.0416282	17.2000000	0.5565684	19.9000000	3.4861164
14.6000000	0.0331674	17.3000000	0.6479917	20.0000000	3.3505578

Table S7: Equilibrium structure of $\mathbf{PA}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.168934	-0.000000	-0.000000
2	6	0	-1.484141	-1.229282	-0.000001
3	6	0	-0.121403	-1.240700	-0.000000
4	6	0	0.590039	0.000000	-0.000000
5	6	0	-0.121404	1.240700	0.000000
6	6	0	-1.484142	1.229282	-0.000000
7	1	0	-3.250883	-0.000000	-0.000000
8	1	0	-2.042016	-2.153987	-0.000001
9	1	0	0.438203	-2.164808	-0.000000
10	1	0	0.438203	2.164808	0.000000
11	1	0	-2.042016	2.153987	0.000000
12	6	0	1.971730	0.000000	0.000000
13	6	0	3.185682	0.000000	0.000001
14	1	0	4.253951	-0.000003	0.000001

Table S8: Equilibrium structure of $\mathbf{PE}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.325076	-1.157995	-0.000002
2	6	0	-2.140152	-0.000002	0.000002
3	6	0	-1.325084	1.157991	0.000002
4	6	0	-0.000001	0.732143	-0.000002
5	6	0	1.325084	-1.157991	-0.000001
6	6	0	0.000001	-0.732143	-0.000004
7	1	0	-1.688788	-2.174457	-0.000002
8	1	0	-3.218573	-0.000005	0.000005
9	1	0	-1.688799	2.174451	0.000005
10	1	0	3.218573	0.000005	0.000004
11	6	0	2.140152	0.000002	0.000002
12	6	0	1.325076	1.157996	0.000001
13	1	0	1.688788	2.174457	0.000003
14	1	0	1.688799	-2.174452	-0.000000

Table S9: Equilibrium structure of $\mathbf{BCB}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.467091	-0.620258
2	6	0	-0.000000	0.719644	0.524720
3	6	0	0.000000	-0.719644	0.524720
4	6	0	-0.000000	-1.467091	-0.620258
5	6	0	-0.000000	-0.704062	-1.793990
6	6	0	0.000000	0.704062	-1.793990
7	1	0	-0.000000	2.546289	-0.641616
8	1	0	0.000000	-2.546289	-0.641616
9	1	0	-0.000000	-1.209759	-2.749778
10	1	0	0.000000	1.209759	-2.749778
11	6	0	0.000000	-0.688207	1.992964
12	1	0	0.000001	-1.436973	2.770781
13	6	0	-0.000000	0.688207	1.992964
14	1	0	-0.000001	1.436973	2.770781

Table S10: Equilibrium structure of $\mathbf{1}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.253279	-0.131617	-0.000001
2	6	0	-1.506464	1.146990	-0.000001
3	6	0	-0.157067	1.181431	0.000001
4	6	0	0.599682	-0.028771	0.000003
5	6	0	-0.041933	-1.303087	0.000000
6	6	0	-1.377131	-1.279928	-0.000001
7	1	0	-2.937626	-0.168226	0.860788
8	1	0	-2.082409	2.063417	-0.000001
9	1	0	0.376617	2.120158	0.000000
10	1	0	0.545604	-2.210549	-0.000000
11	1	0	-2.937625	-0.168226	-0.860791
12	6	0	1.999138	0.035007	0.000001
13	6	0	3.198781	0.085372	-0.000001
14	1	0	4.265089	0.131050	-0.000003

Table S11: Equilibrium structure of $\mathbf{2}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.292655	-0.095934	-0.000001
2	6	0	1.537642	-1.200080	-0.000001
3	6	0	0.096051	-1.289870	0.000000
4	6	0	-0.581679	0.042024	0.000002
5	6	0	0.177951	1.192543	0.000002
6	6	0	1.570120	1.122071	0.000001
7	1	0	3.373364	-0.105477	-0.000003
8	1	0	-0.252212	-1.878705	-0.860947
9	1	0	-0.308632	2.156457	0.000001
10	1	0	2.130357	2.049996	-0.000001
11	6	0	-1.983151	0.073911	0.000001
12	6	0	-3.183065	0.081889	-0.000002
13	1	0	-4.249810	0.097104	-0.000007
14	1	0	-0.252211	-1.878706	0.860948

Table S12: Equilibrium structure of $\mathbf{3}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.200619	0.096162	-0.000009
2	6	0	-1.549075	-1.225458	0.000087
3	6	0	-0.111514	-1.163378	0.000066
4	6	0	0.674674	-0.058158	0.000002
5	6	0	-0.052717	1.159601	-0.000075
6	6	0	-1.456220	1.232795	-0.000082
7	1	0	-3.282467	0.128450	-0.000011
8	1	0	-1.905476	-1.821197	-0.856550
9	1	0	-1.905421	-1.821002	0.856889
10	1	0	0.519951	2.080643	-0.000137
11	1	0	-1.929196	2.203777	-0.000149
12	6	0	2.095771	-0.079388	0.000002
13	6	0	3.290754	-0.077129	0.000003
14	1	0	4.356295	-0.080955	0.000001

Table S13: Equilibrium structure of $\mathbf{4}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.189376	0.135558	0.000004
2	6	0	-1.617209	-1.184932	0.000005
3	6	0	-0.144473	-1.192576	-0.000001
4	6	0	0.573581	-0.027866	-0.000003
5	6	0	-0.128949	1.207204	-0.000003
6	6	0	-1.528902	1.307556	0.000001
7	1	0	-1.996509	-1.766596	0.856422
8	1	0	-1.996521	-1.766610	-0.856396
9	1	0	0.359874	-2.150220	-0.000002
10	1	0	0.458369	2.118663	-0.000003
11	1	0	-2.019018	2.271135	0.000003
12	6	0	1.998026	-0.023100	-0.000003
13	6	0	3.193169	-0.006928	-0.000003
14	1	0	4.258613	0.004135	0.000004

Table S14: Equilibrium structure of $\mathbf{5}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.865002	0.284105	0.000006
2	6	0	-0.527459	0.830039	-0.000000
3	6	0	-0.172413	2.119038	-0.000004
4	6	0	0.364228	-0.336595	0.000005
5	6	0	-0.450074	-1.489538	-0.000002
6	6	0	-1.791074	-1.104350	-0.000000
7	1	0	-2.769656	0.873749	0.000006
8	1	0	0.869275	2.413583	-0.000003
9	1	0	-0.077374	-2.502166	-0.000007
10	1	0	-2.633344	-1.777633	-0.000003
11	6	0	1.742996	-0.306671	0.000001
12	6	0	2.950476	-0.272522	-0.000003
13	1	0	4.017603	-0.252837	-0.000005
14	1	0	-0.916581	2.904258	-0.000003

Table S15: Equilibrium structure of $\mathbf{6}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.218024	1.196274	-0.000005
2	6	0	-1.531176	-0.231450	-0.000002
3	6	0	-2.738779	-0.813494	-0.000007
4	6	0	-0.260188	-0.903429	0.000005
5	6	0	0.759878	0.083384	0.000002
6	6	0	0.142799	1.363621	-0.000004
7	1	0	-1.954683	1.985744	-0.000008
8	1	0	-2.841655	-1.890575	-0.000007
9	1	0	-0.098197	-1.971016	0.000011
10	1	0	0.675023	2.300926	-0.000006
11	6	0	2.126786	-0.189826	0.000006
12	6	0	3.304726	-0.431223	0.000007
13	1	0	4.350404	-0.642935	0.000011
14	1	0	-3.647030	-0.225288	-0.000016

Table S16: Equilibrium structure of $\mathbf{7}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.197601	0.130877	-0.255397
2	6	0	-1.441002	1.278868	-0.117728
3	6	0	-0.126896	1.324138	0.138520
4	6	0	0.558900	0.028592	0.383886
5	6	0	-0.248984	-1.183845	0.172454
6	6	0	-1.586866	-1.125232	-0.085148
7	1	0	-3.253118	0.190207	-0.497026
8	1	0	0.447967	2.237426	0.230919
9	1	0	0.258400	-2.133580	0.281383
10	1	0	-2.171479	-2.027484	-0.191877
11	6	0	1.954895	-0.045974	-0.008296
12	6	0	3.098012	-0.101272	-0.343856
13	1	0	4.119822	-0.151985	-0.641754
14	1	0	0.535659	0.048508	1.511749

Table S17: Equilibrium structure of $\mathbf{8}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.129185	-0.029165	-0.257780
2	6	0	-1.451136	1.198274	-0.129084
3	6	0	-0.127886	1.218273	0.173131
4	6	0	0.614260	-0.041030	0.450253
5	6	0	-0.190053	-1.225300	0.206531
6	6	0	-1.502615	-1.276354	-0.079787
7	1	0	-3.183229	-0.014793	-0.511571
8	1	0	-2.048302	-2.202172	-0.198225
9	6	0	1.997247	-0.075790	-0.002319
10	6	0	3.127237	-0.088211	-0.381108
11	1	0	4.138057	-0.104415	-0.717425
12	1	0	0.427061	2.143055	0.267457
13	1	0	-1.990372	2.119838	-0.291955
14	1	0	0.629577	-0.025696	1.572693

Table S18: Equilibrium structure of $\mathbf{9}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.535592	-0.600989	0.512383
2	6	0	-1.543708	0.644934	-0.088238
3	6	0	-1.679652	1.712170	-0.635571
4	6	0	1.535591	-0.600993	-0.512382
5	6	0	0.619942	-1.626458	-0.322484
6	6	0	-0.619947	-1.626457	0.322484
7	1	0	-2.409536	-0.832982	1.112529
8	1	0	-1.790336	2.654738	-1.122759
9	1	0	0.959212	-2.599656	-0.658418
10	1	0	-0.959219	-2.599654	0.658417
11	6	0	1.543709	0.644930	0.088238
12	6	0	1.679657	1.712166	0.635570
13	1	0	1.790345	2.654734	1.122758
14	1	0	2.409534	-0.832988	-1.112528

Table S19: Equilibrium structure of $\mathbf{10}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.221530	-0.038795	-0.000003
2	6	0	1.558148	-1.274916	-0.000001
3	6	0	0.207585	-1.215142	0.000003
4	6	0	-0.552878	-0.030026	0.000002
5	6	0	0.168812	1.209424	-0.000001
6	6	0	1.536272	1.183754	-0.000003
7	1	0	3.304448	-0.032633	-0.000003
8	1	0	2.106511	-2.206201	-0.000000
9	1	0	-0.384250	2.138697	-0.000002
10	1	0	2.096802	2.106662	-0.000003
11	6	0	-1.904263	-0.058298	0.000003
12	6	0	-3.178364	-0.079883	0.000001
13	1	0	-3.732281	-0.091630	-0.934636
14	1	0	-3.732284	-0.091611	0.934637

Table S20: Equilibrium structure of $\mathbf{11}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.573101	1.563949	-0.200966
2	6	0	-0.652045	1.228572	0.234533
3	6	0	-1.746314	0.579901	0.487251
4	6	0	0.573098	-1.563950	0.200966
5	6	0	1.672265	-0.684805	0.123545
6	6	0	1.672267	0.684802	-0.123544
7	1	0	0.729343	2.547098	-0.630384
8	1	0	-2.453392	0.715017	1.292796
9	1	0	2.642025	-1.130291	0.309195
10	1	0	2.642028	1.130286	-0.309193
11	6	0	-0.652047	-1.228570	-0.234535
12	6	0	-1.746316	-0.579899	-0.487250
13	1	0	-2.453397	-0.715014	-1.292792
14	1	0	0.729337	-2.547098	0.630384

Table S21: Equilibrium structure of $\mathbf{12}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.061395	-0.018089	-0.000002
2	6	0	1.361461	1.194368	0.000006
3	6	0	-0.009078	1.199274	0.000008
4	6	0	-0.719348	-0.040155	0.000002
5	6	0	0.057297	-1.206577	-0.000007
6	6	0	1.410193	-1.259298	-0.000009
7	1	0	3.144123	-0.000023	-0.000005
8	1	0	1.909134	2.125018	0.000010
9	1	0	-0.571109	2.124544	0.000014
10	1	0	-2.539165	-0.106344	-1.639382
11	6	0	-2.195083	-0.088956	-0.623073
12	6	0	-2.195082	-0.088963	0.623075
13	1	0	-2.539165	-0.106368	1.639383
14	1	0	1.965648	-2.186446	-0.000016

Table S22: Equilibrium structure of $\mathbf{13}^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.899726	-0.719507	0.000001
2	6	0	0.757832	-1.481958	-0.000000
3	6	0	-0.392522	-0.693671	-0.000001
4	6	0	-0.392522	0.693670	-0.000001
5	6	0	0.757832	1.481958	-0.000000
6	6	0	1.899726	0.719507	0.000001
7	1	0	2.863138	-1.211597	0.000001
8	1	0	0.766817	-2.560573	0.000000
9	1	0	0.766817	2.560573	-0.000001
10	1	0	2.863138	1.211598	0.000001
11	6	0	-1.588034	-0.000000	-0.000000
12	6	0	-2.978947	0.000000	0.000001
13	1	0	-3.519223	-0.935133	0.000002
14	1	0	-3.519223	0.935133	0.000001

Table S23: Equilibrium structure of $\mathbf{14}^{+}$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.422216	0.692452	-0.000001
2	6	0	-2.422219	-0.692447	-0.000000
3	6	0	-1.085983	-1.147197	0.000000
4	6	0	-0.219480	-0.000002	-0.000000
5	6	0	-1.085978	1.147197	-0.000001
6	1	0	-3.293329	1.327917	-0.000001
7	1	0	-0.758627	-2.175656	0.000000
8	1	0	-0.758618	2.175654	-0.000001
9	6	0	1.121524	-0.000005	-0.000000
10	6	0	2.370017	-0.000004	0.000000
11	1	0	-3.293335	-1.327907	-0.000001
12	6	0	3.682423	0.000003	0.000001
13	1	0	4.237686	0.930486	0.000001
14	1	0	4.237697	-0.930473	0.000001

Table S24: Equilibrium structure of **PA-1**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.237301	-0.077434	-0.056084
2	6	0	1.533041	1.159886	-0.004478
3	6	0	0.169158	1.160515	0.001940
4	6	0	-0.595105	-0.043204	-0.012797
5	6	0	0.053884	-1.271564	-0.028890
6	6	0	1.439086	-1.232281	-0.062097
7	1	0	3.314319	-0.136048	-0.152322
8	1	0	2.096872	2.081373	0.010899
9	1	0	-0.365845	2.099600	0.021636
10	1	0	-0.492914	-2.203486	-0.023444
11	1	0	1.984295	-0.811448	1.034943
12	6	0	-2.010079	0.022996	0.000218
13	6	0	-3.205135	0.085921	0.010471
14	1	0	-4.269641	0.140991	0.018591

Table S25: Equilibrium structure of **PA-2**$^{+}$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.274581	-0.079345	-0.025554
2	6	0	-1.476566	-1.216659	-0.063317
3	6	0	-0.074144	-1.240522	-0.063257
4	6	0	0.595610	0.027442	-0.008669
5	6	0	-0.185265	1.167795	0.010219
6	6	0	-1.589642	1.116528	0.000047
7	1	0	-3.353282	-0.135502	-0.021780
8	1	0	-0.826855	-1.425277	1.031925
9	1	0	0.305204	2.130635	0.034835
10	1	0	-2.147773	2.043120	0.019875
11	6	0	2.010213	0.060364	-0.001265
12	6	0	3.206898	0.074783	0.000016
13	1	0	4.272654	0.094624	0.001420
14	1	0	0.474919	-2.169915	-0.155591

Table S26: Equilibrium structure of **PA-3**$^{+}$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.215277	0.034618	-0.019948
2	6	0	-1.529812	-1.217445	-0.049858
3	6	0	-0.125261	-1.163219	-0.068653
4	6	0	0.656923	-0.004682	-0.013530
5	6	0	-0.075312	1.178055	0.007275
6	6	0	-1.481023	1.189409	0.003488
7	1	0	-3.295382	0.040952	-0.019818
8	1	0	-2.048328	-2.161162	-0.170788
9	1	0	-0.886214	-1.344056	1.043715
10	1	0	0.467226	2.114147	0.032447
11	1	0	-1.989717	2.142945	0.021646
12	6	0	2.072089	-0.049996	-0.006560
13	6	0	3.267578	-0.080794	-0.003326
14	1	0	4.332991	-0.108500	-0.000525

Table S27: Equilibrium structure of **PA-4**$^{+}$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.177455	0.062915	-0.060378
2	6	0	-1.561452	-1.200782	-0.045631
3	6	0	-0.136526	-1.215592	-0.024848
4	6	0	0.559536	-0.025847	-0.010403
5	6	0	-0.140661	1.215730	-0.006857
6	6	0	-1.512680	1.280861	-0.015854
7	1	0	-1.985643	-0.693505	1.049813
8	1	0	-2.142255	-2.107820	-0.162323
9	1	0	0.379856	-2.164340	-0.026886
10	1	0	0.436433	2.130841	0.011410
11	1	0	-2.044682	2.221279	-0.006123
12	6	0	1.979575	-0.017751	0.002753
13	6	0	3.175523	0.000409	0.013252
14	1	0	4.241126	0.013894	0.021907

Table S28: Equilibrium structure of **PA-8**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.623666	-0.693774	-0.486555
2	6	0	-0.613702	-1.415805	0.036335
3	6	0	0.477135	-0.727820	0.757217
4	6	0	0.326629	0.700361	0.852263
5	6	0	-0.677534	1.451439	0.263664
6	6	0	-1.663462	0.731231	-0.365386
7	1	0	-2.432766	-1.189604	-1.003060
8	1	0	-0.586282	-2.494778	-0.022982
9	1	0	0.908111	-1.254902	1.606676
10	1	0	-0.688157	2.530437	0.308450
11	1	0	-2.496344	1.262391	-0.809182
12	6	0	1.588568	-0.170868	-0.091253
13	6	0	2.512992	0.220342	-0.756313
14	1	0	3.333681	0.575814	-1.339738

Table S29: Equilibrium structure of **PA-10**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.055180	0.487253	-0.000024
2	6	0	1.802605	-0.881668	-0.000021
3	6	0	0.512278	-1.398369	-0.000004
4	6	0	-0.505316	-0.460485	0.000009
5	6	0	-0.194094	0.877820	-0.000018
6	6	0	1.033763	1.452202	0.000004
7	1	0	3.078393	0.838366	-0.000047
8	1	0	2.640508	-1.563411	-0.000027
9	1	0	0.316501	-2.460223	0.000005
10	1	0	-4.020694	0.553321	-0.000060
11	6	0	-3.028043	0.153432	0.000048
12	6	0	-1.933263	-0.392471	0.000034
13	1	0	-1.704875	1.093258	-0.000052
14	1	0	1.231507	2.512404	0.000012

Table S30: Equilibrium structure of **1-6**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.463276	-0.259234	0.293636
2	6	0	1.482692	0.990873	-0.064186
3	6	0	0.135852	1.146811	-0.025399
4	6	0	-0.704423	-0.009572	-0.046168
5	6	0	0.096917	-1.201146	-0.142823
6	6	0	1.372050	-0.885409	-0.269026
7	1	0	3.366999	-0.116954	-0.287938
8	1	0	2.112146	1.786755	-0.438893
9	1	0	-0.282647	2.137998	-0.132968
10	1	0	-0.274909	-2.211247	-0.046165
11	1	0	2.626769	-0.386193	1.364930
12	6	0	-2.087224	-0.000023	0.041363
13	6	0	-3.291224	0.011977	0.108111
14	1	0	-4.355850	0.023973	0.167989

Table S31: Equilibrium structure of **2-5**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.894820	0.330710	-0.504424
2	6	0	-0.740729	0.995409	-0.426792
3	6	0	0.060456	1.602464	0.509411
4	6	0	0.376250	-0.118752	0.244756
5	6	0	-0.496615	-1.232985	0.465593
6	6	0	-1.742705	-1.028352	-0.031916
7	1	0	-2.824299	0.783684	-0.818133
8	1	0	1.015579	2.041636	0.254115
9	1	0	-0.112075	-2.169909	0.838542
10	1	0	-2.536644	-1.758355	-0.054608
11	6	0	1.708065	-0.241641	-0.080102
12	6	0	2.880898	-0.355873	-0.358309
13	1	0	3.912764	-0.465405	-0.608615
14	1	0	-0.360134	1.862481	1.479389

Table S32: Equilibrium structure of **2-7**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.260113	-0.123365	-0.091669
2	6	0	-1.591682	1.118738	-0.020806
3	6	0	-0.226089	1.182551	0.051493
4	6	0	0.570374	-0.008236	0.088759
5	6	0	-0.127477	-1.291916	0.013191
6	6	0	-1.498645	-1.245954	-0.063730
7	1	0	-3.339769	-0.164170	-0.158355
8	1	0	-2.170914	2.031659	-0.034236
9	1	0	0.286923	2.132765	0.081447
10	1	0	0.456316	-2.203506	0.035709
11	1	0	0.258436	-0.531894	1.167618
12	6	0	1.994496	0.042886	-0.011014
13	6	0	3.183234	0.091670	-0.113720
14	1	0	4.244419	0.136914	-0.207210

Table S33: Equilibrium structure of **3-5**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.096123	0.033788	-0.024152
2	6	0	-1.482160	-1.428139	0.132417
3	6	0	-0.242920	-0.906400	-0.209299
4	6	0	0.659421	0.044033	-0.088649
5	6	0	-0.049944	1.312514	0.026803
6	6	0	-1.445322	1.229225	0.043547
7	1	0	-3.143830	-0.038193	-0.285847
8	1	0	-1.981375	-2.061673	-0.599206
9	1	0	-1.587893	-1.805571	1.154902
10	1	0	0.518519	2.223398	0.141068
11	1	0	-2.039409	2.132875	0.042255
12	6	0	2.060871	-0.104515	-0.015540
13	6	0	3.250010	-0.206106	0.043461
14	1	0	4.310990	-0.297238	0.095297

Table S34: Equilibrium structure of **4-6**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.911488	0.101823	-0.170853
2	6	0	-1.791956	-1.247865	0.128303
3	6	0	-0.221673	-1.088310	-0.056337
4	6	0	0.553642	0.043179	0.029336
5	6	0	-0.051237	1.325270	0.047107
6	6	0	-1.484645	1.327291	-0.042000
7	1	0	-2.064444	-1.542739	1.146662
8	1	0	-2.126949	-1.966270	-0.617837
9	1	0	0.205705	-2.030630	-0.373631
10	1	0	0.503212	2.244763	0.154832
11	1	0	-2.102160	2.211046	0.044098
12	6	0	1.970671	-0.076350	0.008365
13	6	0	3.163189	-0.163934	-0.001325
14	1	0	4.225614	-0.242793	-0.009715

Table S35: Equilibrium structure of **7-8**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.628373	-0.837906	-0.437515
2	6	0	0.613738	-1.416695	0.212093
3	6	0	-0.449487	-0.751099	0.865226
4	6	0	-0.394022	0.721303	0.816860
5	6	0	0.708544	1.343567	0.129992
6	6	0	1.663930	0.596231	-0.476481
7	1	0	2.419490	-1.413172	-0.900221
8	1	0	-1.063567	-1.245133	1.607344
9	1	0	0.758626	2.422337	0.126368
10	1	0	2.488976	1.080994	-0.979949
11	6	0	-1.456972	0.008573	-0.151827
12	6	0	-2.386310	-0.013652	-0.921469
13	1	0	-3.201279	-0.035382	-1.612785
14	1	0	-0.969011	1.288418	1.537974

Table S36: Equilibrium structure of **7-9**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.164607	0.151052	-0.301802
2	6	0	-1.256895	1.174184	-0.111951
3	6	0	-0.161371	1.697151	0.091577
4	6	0	0.594980	-0.148468	0.550494
5	6	0	-0.286366	-1.247366	0.186176
6	6	0	-1.630178	-1.119746	-0.062110
7	1	0	-3.160170	0.315273	-0.686244
8	1	0	0.564560	2.450358	0.315191
9	1	0	0.196850	-2.209040	0.063169
10	1	0	-2.245903	-1.993685	-0.218651
11	6	0	1.908416	-0.141497	0.030373
12	6	0	3.018451	-0.135562	-0.422110
13	1	0	4.009859	-0.139428	-0.815683
14	1	0	0.500223	0.198035	1.578330

Table S37: Equilibrium structure of **8-10**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.209373	-0.038429	-0.029796
2	6	0	-1.518762	1.176045	-0.014341
3	6	0	-0.146021	1.205315	0.014738
4	6	0	0.555799	-0.029002	0.005653
5	6	0	-0.185522	-1.207831	0.021666
6	6	0	-1.540110	-1.266922	-0.012218
7	1	0	-3.291200	-0.033064	-0.046664
8	1	0	-2.080807	-2.202814	-0.018887
9	6	0	2.021845	-0.062210	-0.073239
10	6	0	3.229680	-0.081737	-0.070014
11	1	0	4.298400	-0.103822	-0.045429
12	1	0	0.404914	2.135558	0.031107
13	1	0	-2.071198	2.103893	-0.023078
14	1	0	1.494680	-0.071121	1.048259

Table S38: Equilibrium structure of **9-11**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.086269	-1.346559	-0.375322
2	6	0	0.147764	-1.457869	0.187289
3	6	0	1.258198	-1.303413	0.701685
4	6	0	-0.100591	1.603919	0.257004
5	6	0	-1.355943	1.076736	0.275238
6	6	0	-1.814321	-0.181654	-0.208810
7	1	0	-1.496359	-2.166658	-0.950280
8	1	0	2.081756	-1.353729	1.380862
9	1	0	-2.136331	1.761003	0.582398
10	1	0	-2.850005	-0.206857	-0.527507
11	6	0	1.083111	1.010020	-0.225328
12	6	0	2.097865	0.463545	-0.610856
13	1	0	3.010858	0.141809	-1.061827
14	1	0	0.011195	2.636080	0.570960

Table S39: Equilibrium structure of **10-12**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.116719	-0.311288	0.065519
2	6	0	1.660662	1.003803	0.107284
3	6	0	0.311875	1.296264	0.029066
4	6	0	-0.587458	0.235851	-0.121613
5	6	0	-0.088887	-1.051341	-0.139829
6	6	0	1.229887	-1.381459	-0.065682
7	1	0	3.177558	-0.511940	0.127251
8	1	0	2.372181	1.812548	0.189187
9	1	0	-0.039249	2.318539	0.063784
10	1	0	-3.412520	-1.279463	0.605120
11	6	0	-2.795099	-0.475594	0.241808
12	6	0	-2.047812	0.459917	-0.177755
13	1	0	-2.477695	1.406415	-0.514637
14	1	0	1.580410	-2.403013	-0.103488

Table S40: Equilibrium structure of **10-13**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.991605	-0.552890	0.160679
2	6	0	-0.970073	-1.460061	-0.049999
3	6	0	0.233238	-0.844761	-0.337667
4	6	0	0.453797	0.511805	-0.330184
5	6	0	-0.579201	1.432296	-0.047508
6	6	0	-1.804017	0.857482	0.148920
7	1	0	-2.986060	-0.931859	0.359071
8	1	0	-1.120151	-2.528444	-0.026376
9	1	0	-0.409971	2.497702	-0.005190
10	1	0	-2.663137	1.485305	0.338009
11	6	0	1.728061	0.167286	-0.029788
12	6	0	2.963389	-0.118093	0.255473
13	1	0	3.215645	-0.882962	0.979113
14	1	0	3.762133	0.401875	-0.264181

Table S41: Equilibrium structure of **11-BCB**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.583264	-1.503516	-0.180383
2	6	0	0.615247	-1.042354	0.182946
3	6	0	1.844167	-0.611836	0.411103
4	6	0	-0.583265	1.503516	0.180382
5	6	0	-1.743610	0.680752	0.094412
6	6	0	-1.743610	-0.680753	-0.094412
7	1	0	-0.671254	-2.508247	-0.576998
8	1	0	2.574777	-0.939717	1.136500
9	1	0	-2.698759	1.171302	0.222989
10	1	0	-2.698758	-1.171303	-0.222988
11	6	0	0.615246	1.042354	-0.182946
12	6	0	1.844167	0.611836	-0.411102
13	1	0	2.574776	0.939716	-1.136500
14	1	0	-0.671255	2.508247	0.576996

Table S42: Equilibrium structure of **12-BCB**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.981187	-0.226989	0.091602
2	6	0	-1.461992	1.094636	0.143977
3	6	0	-0.131653	1.344565	0.004530
4	6	0	0.715640	0.235019	-0.308301
5	6	0	0.148204	-1.027084	-0.372789
6	6	0	-1.181146	-1.325010	-0.134137
7	1	0	-3.041647	-0.373611	0.250941
8	1	0	-2.145215	1.911096	0.328953
9	1	0	0.277058	2.342430	0.081782
10	1	0	1.958668	-1.020848	1.622718
11	6	0	1.923158	-0.538952	0.662669
12	6	0	2.223598	0.225386	-0.308596
13	1	0	2.992597	0.783862	-0.812143
14	1	0	-1.569191	-2.332354	-0.145989

Table S43: Equilibrium structure of **BCB-PE**$^+$ optimized at the ωB97X-D/aug-cc-pVTZ level of theory

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.802411	1.336598	0.001105
2	6	0	0.370044	0.747038	0.167207
3	6	0	0.744158	-0.916162	-0.351186
4	6	0	-0.348316	-1.175586	0.402844
5	6	0	-1.710307	-0.849261	-0.039519
6	6	0	-1.951150	0.455593	-0.192902
7	1	0	-0.889137	2.414868	-0.030248
8	1	0	-0.209438	-1.573225	1.410977
9	1	0	-2.449898	-1.629272	-0.145796
10	1	0	-2.918782	0.852439	-0.458609
11	6	0	2.063869	-0.499710	-0.274154
12	1	0	2.974695	-1.002728	-0.554331
13	6	0	1.806069	0.790303	0.175263
14	1	0	2.460823	1.605037	0.446066

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