Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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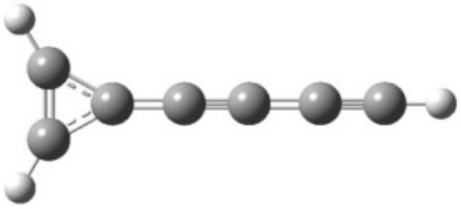
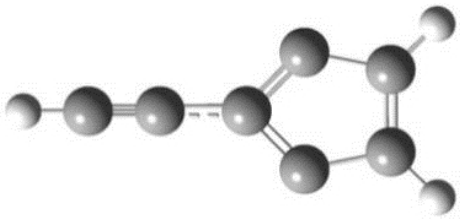
Supplementary material:

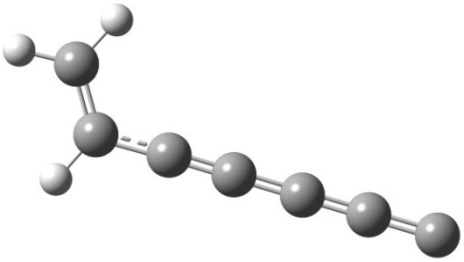
Table S1. Energies in kJ mol^{-1}, relative to the most stable cation and neutral species of the cation and neutral isomers calculated with MP2/cc-pVDZ basis set. D^- energy (relative to C^-) is calculated in DFT using B3LYP functional and cc-pVDZ basis set.



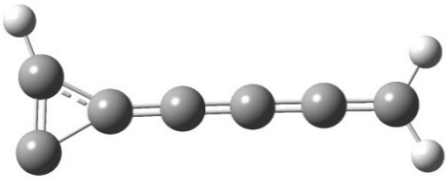
A^+ (0)
$A^\bullet$ (160)



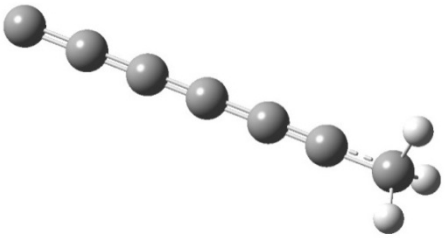
D^+ (245)
$D^\bullet$ (68)
D^- (170)



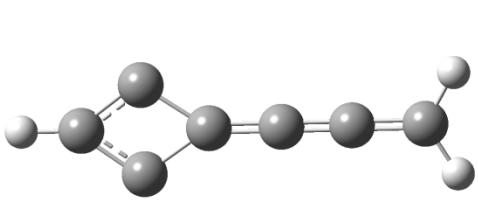
G^+ (213)
$G^\bullet$ (239)

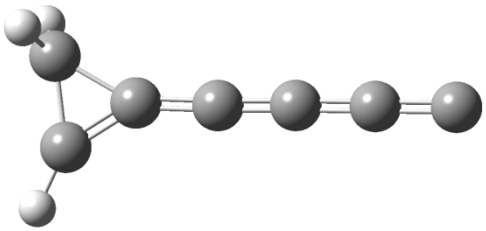


H^+ (236)
$H^\bullet$ (186)



I^+ (383)
$I^\bullet$ (123)





K^+ (187) **L^+ (487)**

$K^\bullet$ (210) **$L^\bullet$ (281)**

Table S2. Electronic excitation energies E_{cal} (eV) and oscillator strength (f) of the dipole allowed electronic transitions for $C_7H_3^+$ and $C_7H_3^\bullet$ isomers, listed in Table S1, are calculated by the CASPT2 method.

Ground state	E_{cal}	f	Excited State
A^+			
X $^1A_1$ (C_{2V})	4.13	0.403	1 $^1A_1$
	5.99	0.005	2 $^1A_1$
$A^\bullet$			
X $^2B_1$ (C_{2V})	1.72	0.002	1 $^2A_2$
	4.76	0.131	3 $^2B_1$
D^+			
X $^1A_1$ (C_{2V})	5.11	0.017	1 $^1A_1$
	5.90	0.011	2 $^1A_1$
$D^\bullet$			
X $^2A_2$ (C_{2V})	2.49	0.002	2 $^2B_1$
	3.28	0.003	1 $^2A_2$
	4.87	0.026	4 $^2B_1$
F^+			
X $^1A_1$ (C_{2V})	5.46	0.125	**1** $^1A_1$
	6.15	0.009	**2** $^1A_1$

F•

X $^2A_2$ (C_{2V})	1.15	0.031	**1** $^2B_1$
	4.44	0.042	**2** $^2B_1$
	5.64	0.187	**3** $^2B_1$

G$^+$

X $^1A'$ (C_S)	2.60	0.004	**1** $^1A'$
	2.69	0.155	**2** $^1A'$
	4.31	0.348	**3** $^1A'$

G•

X ^2A (C_1)	4.536	0.002	**9** ^2A

H$^+$

X $^1A'$ (C_S)	2.59	0.133	**1** $^1A'$
	4.15	0.292	**2** $^1A'$
	4.33	0.024	**3** $^1A'$
	5.48	0.359	**4** $^1A'$
	5.62	0.557	**5** $^1A'$

H•

X ^2A (C_S)	3.57	0.002	**3** ^2A
	4.17	0.005	**4** ^2A

I$^+$

X $^1A'$ (C_S)	2.94	0.029	**3** $^1A'$
	3.06	0.001	**4** $^1A'$
	4.18	0.015	**7** $^1A'$

I•

X $^2A'$ (C_S)	2.51	0.012	**2** $^2A'$
	3.08	0.014	**3** $^2A'$
	3.87	0.008	**5** $^2A'$

K^+

X $^1A_1$ (C_{2V})	4.36	0.54	1 $^1A_1$
	5.27	0.023	2 $^1A_1$
	5.81	0.70	3 $^1A_1$

Table S3. Ground state vibrations (cm^{-1}) of isomer $\mathbf{B}^+$ calculated at the MP2 /cc-pVDZ level:

Symm. a_1 $\nu_1 - \nu_9$: 3442, 3157, 2543, 2245, 2087, 1531, 1414, 1049, 549

b_1 $\nu_{10} - \nu_{16}$: 1043, 688, 618, 553, 331, 201, 77

b_2 $\nu_{17} - \nu_{24}$: 3275, 1026, 727, 509, 436, 264, 191, 76.