Supplementary materials

Table of Contents

Experimental Section

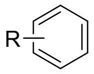
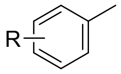
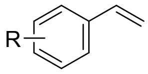
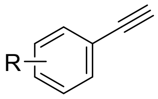
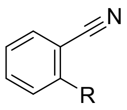
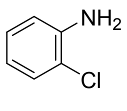
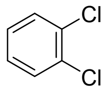
Reagents

All chemicals of benzene derivatives of analytical grade were purchased from Aladdin Biochemical Technology Co., Ltd. (Shanghai, China), and used directly without further purification. High pure nitrogen gas (99.999%) provided by Xi'an Tenglong Chemical Co., Ltd. (Xi'an, China) was used as the discharge gas and carrier gas.

Gas discharge and Mass Spectrometry

Mass spectrometry experiments were performed with a commercial linear ion trap mass spectrometer (LTQ XL; Thermal Fisher, San Jose, CA) equipped with an Ion Max APCI source. The sample was introduced into the corona discharge zone by a headspace approach as depicted in Fig S1. Specifically, the pure liquid sample in a wash bottle was flushed by N_2 gas, and the sample vapor was carried by the nitrogen gas to the APCI ion source inlet. The flow rate of the carrier gas was optimized to maximize the total ion current and the abundance of precursor ions, and was set at 0.7 L/min for all the experiment. Then the benzene derivatives were carried by N_2 gas to the ion source plasma region, where they subjected to ionization, fragmentation and chemical reactions. Note that N_2 was used as the carrier gas to keep consistency with the N_2 atmosphere in the APCI source, which was created by the sheath gas and auxiliary gas both being N_2. The ionized sample formed in the corona discharge region may react with the background N_2 gas, and the ion-molecule reaction product was on-line monitored by mass spectrometry. In positive ion mode, mass spectra were acquired with the Xcalibur (version 4.0 QF2) software and were collected under automatic gain control. The mass spectrometry operating parameters were as follows: source temperature, 200°C; sheath gas, 14 arbitrary units; auxiliary gas, 12 arbitrary units; corona current, 4 uA; capillary voltage, 40 V; capillary temperature, 200°C; tube lens, 90 V. All spectra were collected under automatic gain mode, where per spectrum was set 3 microscans at 100 ms maximum ion injection time.

Table S1 Summary of benzene derivatives and the related ions

Benzene derivatives	R	Isomer	m/z Ar$^+$	m/z ArN$_2^+$	ArN$_2^+$ abundance[a]
	H (**1**)		77	105	18
	F (**2**)				3
	Cl (**3**)				22
	Br (**4**)				74
	I (**5**)				220
	Cl	*o*- (**6**)	91	119	0
		p- (**7**)			
	Br	*o*- (**8**)			
	Cl	*o*- (**9**)	103	131	0
		p- (**10**)			
	Br	*o*- (**11**)			
	F	*o*- (**12**)	101	129	23
	Cl	*o*- (**13**)			288
		p- (**14**)			160
	Br	*o*- (**15**)			367
	Cl (**16**)		102	130	325
	Br (**17**)				409
	(**18**)		92	120	0
	(**19**)		111/113	139/141	221

[a] Relative product abundance refers to the abundance ratio of the $[ArN_2]^+$ and the corresponding molecular radical cation M$^+$. Taking the parent benzene for example, it corresponds to the abundance ratio of m/z, 105/78. Note

that for benzene derivatives **6**-**11** and **18**, the corresponding ArN_2^+ cations were not observed on mass spectrometry

Reaction process details

Under atmospheric pressure of N_2, the highly energetic electrons initially impact and ionize N_2 molecules due to their high concentration, giving rise to N_2^+ (eq S1).the benzene molecule was ionized by the reagent N_2^+ ion leading to benzene radical cation ($C_6H_6^+(v)$)(eq S2); Due to the excess internal energy after the charge transfer between N_2 (15.58 eV) and benzene (9.24 eV) is higher than the C-H bond dissociation energy (De) of 4.89 eV, causing C-H bond breakage for $C_6H_5^+$ formation (Ph^+)(eq S3), which subsequently bind to a N_2 giving rise to PhN_2^+ (eqs S4-5).

$$e^* + N_2 \rightarrow N_2^+ + 2e \qquad S1$$

$$C_6H_6 + N_2^+ \rightarrow C_6H_6^+(v) + N_2 \qquad S2$$

$$C_6H_6^+(v) \rightarrow C_6H_5^+(v) + H \qquad S3$$

$$C_6H_5^+(v) + N_2 \rightarrow C_6H_5^+ + N_2 \qquad S4$$

$$C_6H_5^+ + N_2 \rightarrow C_6H_5N_2^+ \qquad S5$$

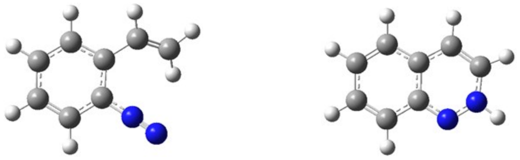
According to the basic quasi-equilibrium theory (QET S6), there would be an exponential increase for the fragmentation rate constant when the C-H bond is replaced with a weaker C-X bond. Equation S6 is basically a simplified form of Rice–Ramsperger–Kassel (RRK) theory, which for energized molecular ions at relatively low pressure, can be simplified to equation S6. It is often used in the field of mass as a rule of thumb to qualitatively describe dissociation or rearrangement of energized molecule or ions spectrometry. At high pressure or with less excess energy, the energized molecular ions may approach toward equilibrium, which would make equation S6 less accurate. That is why an effective number of oscillators are used, rather than the actual vibrational degrees of freedom. The simplified QET is often applied in the field of mass spectrometry to qualitatively explain experiment observation. On the other hand, in practice, the number of vibration freedom has to be replaced by an effective number, in order to better fit the experimental result. The effective number is usually in the range of 1/4 ~ 2/3 of the actual vibrational degrees of freedom. For tolyl cation ($C_7H_7^+$), the effective number of 15 corresponds to an effective factor ca. 2/5 (15/32).

$$k = v \times e^{-(s-1)^{E^{\ddagger}} / E_{int}} \qquad \text{S6}$$

Scheme

Density functional theory (DFT) calculations

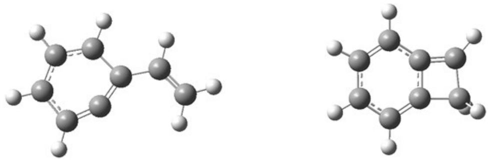
The structures involved in this study were optimized by B3LYP (Becke, 3-parameter, Lee–Yang–Parr) in combination with the double-zeta polarized basis set 6-31G*, and the nature of the optimized structures as a minimum or transition state was verified by frequency calculations. The energetics were calculated at the same theory level based on the optimized geometries. All calculations were performed with the Gaussian09 package.



0.00 -1.73

(**S1**) (**20**)

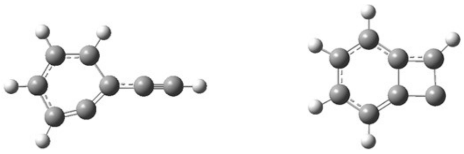
Fig. S2. Structures and energetics (in eV) of ArN_2^+ and the possible protonated cinnoline iosomers (**20**) as shown in **Scheme S1**.



0.00 -1.52

(**25**) (**26**)

Fig. S3. Structures and energetics (in eV) of Ar^+ (**25**) and the ring-closing isomers (**26**) as shown in **Scheme S2**.



0.00 0.55

(**S2**) (**S3**)

Fig. S4. Structures and energetics (in eV) of Ar^+ and the ring-closing isomers generated from 2-Chlorophenylacetylene (Cl-Ph-C_2H) (**13**)

0.00 0.69

(**S4**) (**21**)

Fig. S5. Structures and energetics (in eV) of ArN_2^+ and the possible ring-closing iosomer (**21**) generated from 2-chlorophenylacetylene (**13**) as shown in **Scheme S1**.

Spectra

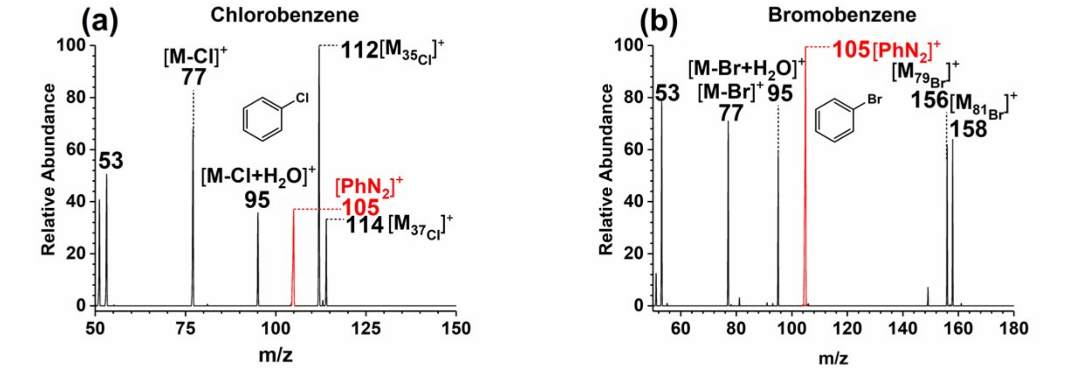


Fig. S6. Atmospheric pressure corona discharge ionization mass spectra of: (a) PhCl; (b) PhBr. (C)PhF. (d) correlation of the C-X bond dissociation energy and abundance of ions relative to the respective molecular ion (M^+): $I_r = I_{105}/I_M$ and $I_t = (I_{77} + I_{95} + I_{105})/I_M^+$, where I_{77}, I_{105}, and I_{95} refer to the relative abundance of $C_6H_5^+$, $C_6H_5N_2^+$ and $C_6H_5OH_2^+$, respectively, on the mass spectra.

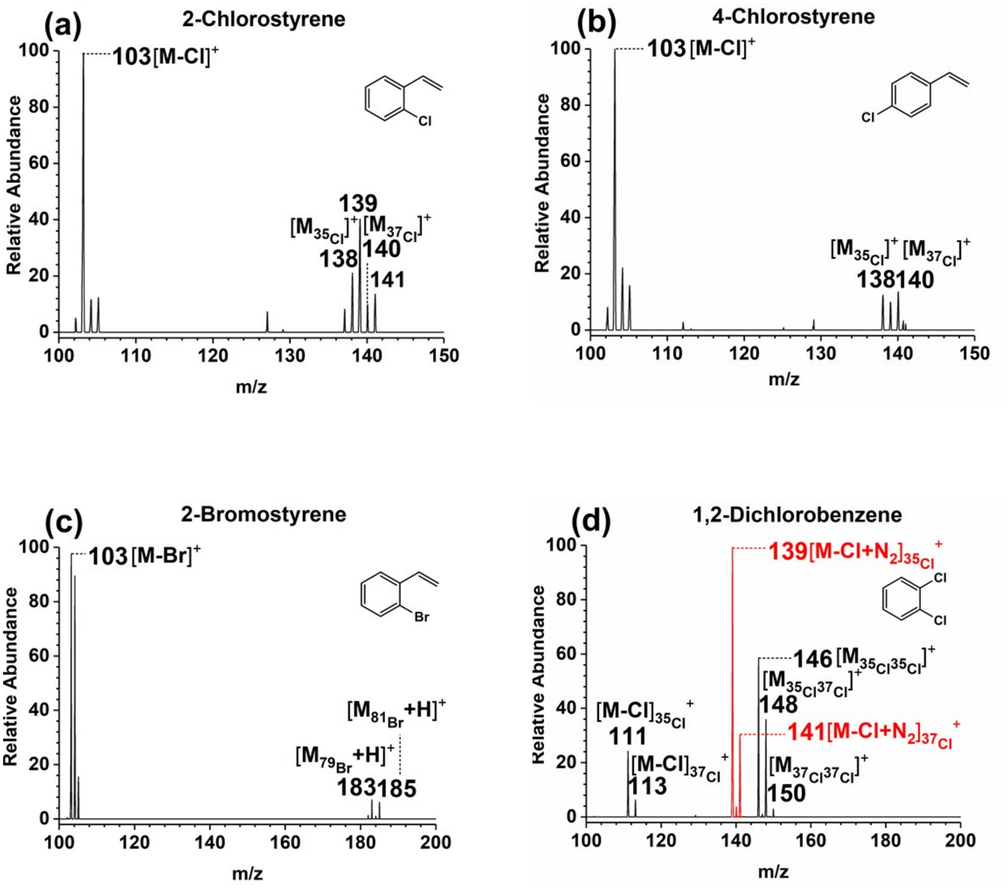


Fig. S7. Atmospheric pressure corona discharge ionization mass spectra of (a) 2-chlorostyrene; (b) 4-chlolostyrene. (c) 2-bromostyrene; (d) 1,2-dichlorobenzene.

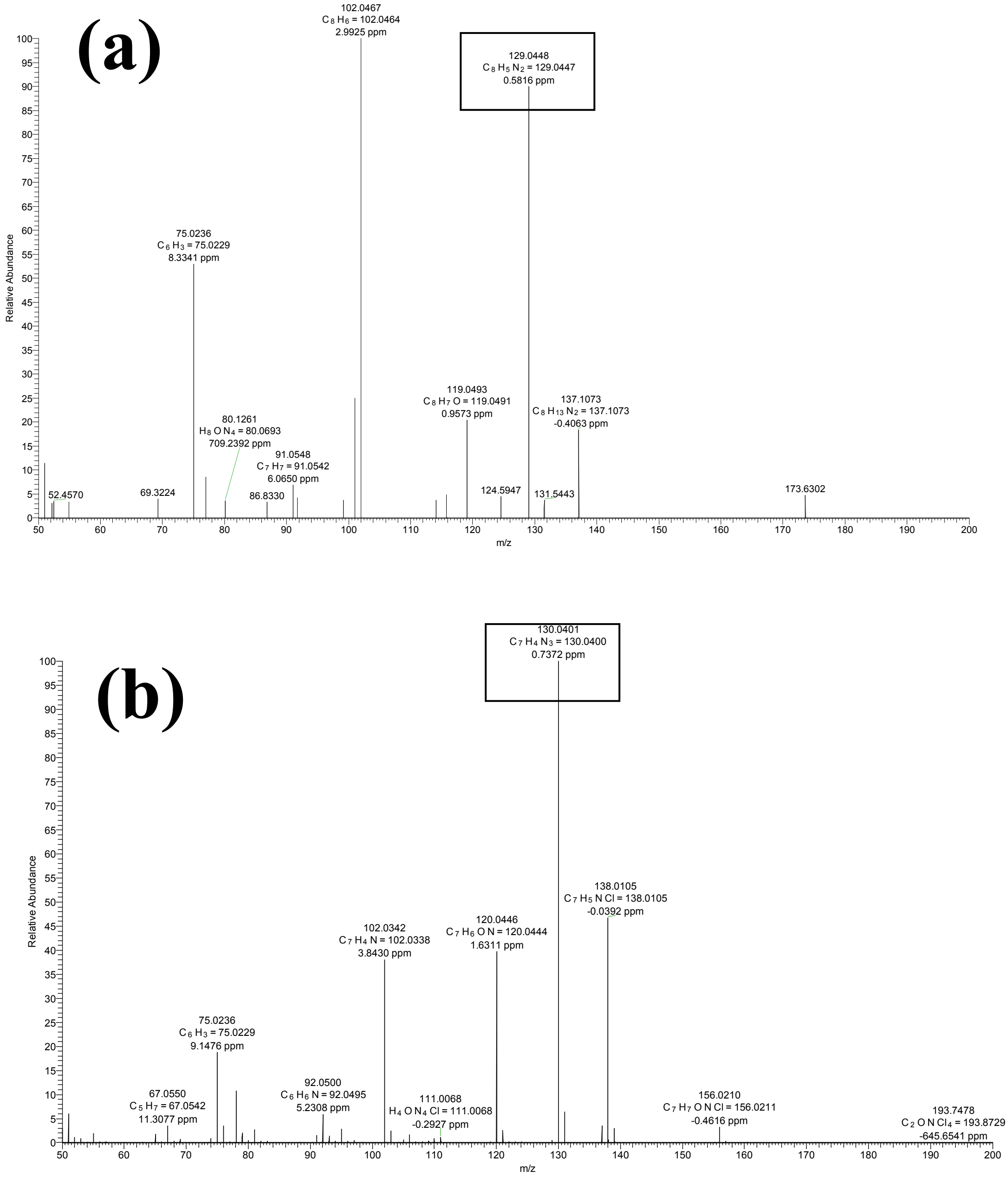


Fig. S8. MS/MS scan to obtain the aryldiazonium cations from the corresponding protonated molecular precursor ions of: (a) 2-chlorophenylacetylene; (b) 2-chlorobenzonitrile. The mass spectra were obtained from QE Orbitrap mass spectrometer by applying 70% collision energy in the HCD cell with background gas of N_2. The peaks (marked by red boxes) at m/z 129 and 130 correspond to the arylium ions from 2-chlorophenylacetylene and 2-chlorobenzonitrile, respectively.

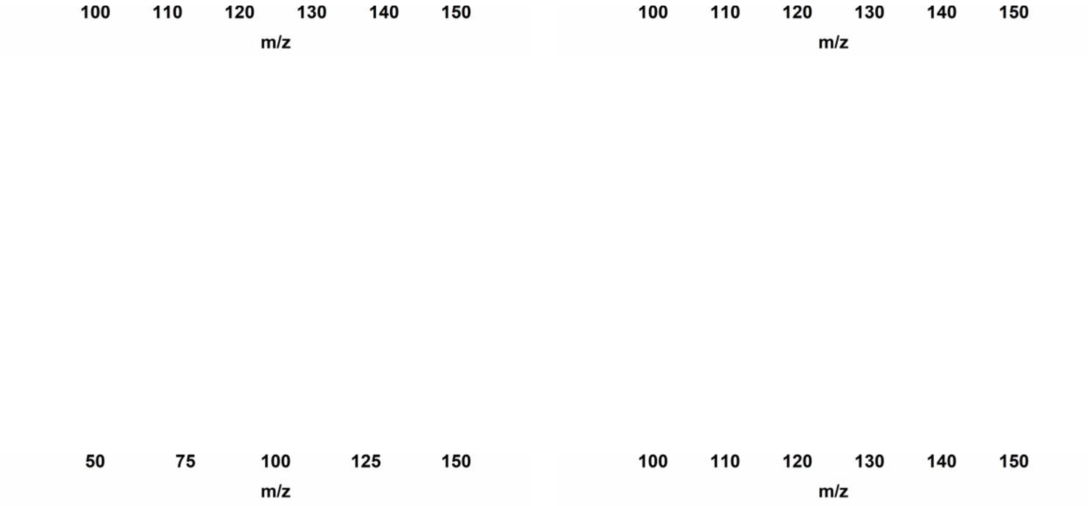


Figure S9. Positive ion mode full-scan APCI mass spectra of (a) 2-chlorophenylacetylene. (b) 4-chlorophenylacetylene. (c) 2- fluorophenylacetylene. (d) 2-chlorobenzonitrile.

Figure S10. Positive ion mode full-scan APCI mass spectra of (a) 2-bromotoluene; (b) 2-chloroaniline.

Table S2. Cartesian coordinate and frequencies of structure **S1** as in Figure S2

E= -418.261151437 Hartree

C	1.17599900	1.44162400	-0.13273200
C	-0.06370100	0.78712700	-0.10481900
C	0.01380000	-0.63282600	0.00344700
C	1.22116100	-1.36259700	0.13981100
C	2.40529200	-0.65215900	0.14833800
C	2.37760500	0.74729800	0.00127100
H	1.18272000	2.52178100	-0.23522600
H	1.19870800	-2.44415400	0.21746100
H	3.34830000	-1.17662600	0.25305600
H	3.31150800	1.30030600	-0.00577700
N	-1.12654600	-1.37842600	-0.11111500
N	-2.02940600	-2.02415700	-0.23836100
H	-3.32290500	1.90641900	0.30611300
C	-1.30582300	1.55452200	-0.19924600
C	-2.46099800	1.25592600	0.41212900
H	-1.22624200	2.47755000	-0.76832900
H	-2.58043100	0.39932100	1.06983900

Frequencies --	88.0523	137.9376	159.0603
Frequencies --	202.1565	232.2290	376.4302
Frequencies --	392.9753	441.4029	512.0737
Frequencies --	525.7135	566.0940	606.9398

Frequencies --	643.9780	717.9630	750.2007
Frequencies --	781.1020	829.0046	901.0413
Frequencies --	987.5694	1002.4138	1015.9199
Frequencies --	1034.8593	1043.2728	1058.4481
Frequencies --	1128.2059	1182.9877	1207.6127
Frequencies --	1237.2618	1291.7419	1334.9673
Frequencies --	1380.3378	1448.7072	1475.6619
Frequencies --	1512.9444	1585.1341	1629.8443
Frequencies --	1690.8800	2327.2495	3172.4308
Frequencies --	3185.2822	3213.0426	3222.5120
Frequencies --	3226.4506	3237.7070	3264.3267

Table S3. Cartesian coordinate and frequencies of structure **20** as in Figure S2

E= -418.324598089 Hartree

C	1.26191100	1.42791600	-0.00000400
C	0.01595700	0.75899600	-0.00000200
C	0.00208900	-0.68849700	-0.00001100
C	1.22313200	-1.42031900	0.00000700
C	2.40979500	-0.73180200	0.00000600
C	2.42742200	0.69262000	-0.00000400
H	1.28634300	2.51262400	-0.00000100
H	1.17751900	-2.50342300	0.00001100
H	3.35043100	-1.27201100	0.00001000
H	3.38385900	1.20552100	-0.00000400

N	-1.14223400	-1.39460000	-0.00000700
N	-2.25441800	-0.70873300	0.00000100
H	-3.38760700	1.03633000	0.00001100
C	-1.23466800	1.40809700	0.00000400
C	-2.37855100	0.64386100	0.00000400
H	-1.30683800	2.49019600	0.00001000
H	-3.08966200	-1.29113100	-0.00000200

```
Frequencies --    177.1213        180.2202        380.3574

Frequencies --    398.7835        463.2714        488.9408

Frequencies --    517.2333        532.4596        637.3022

Frequencies --    640.7718        764.4178        769.1817

Frequencies --    783.9573        832.5028        833.0857

Frequencies --    877.6602        913.0504        974.7162

Frequencies --    988.9562       1008.3650       1034.1993

Frequencies --   1039.3998       1080.6295       1165.8303

Frequencies --   1178.7350       1196.8659       1266.2437

Frequencies --   1290.5151       1318.0646       1367.7193

Frequencies --   1430.3554       1454.0172       1487.5109

Frequencies --   1543.4416       1552.3613       1610.9832

Frequencies --   1633.7182       1659.3203       3210.7800

Frequencies --   3219.9916       3226.8655       3229.5389

Frequencies --   3237.4611       3255.7748       3549.3934
```

Table S4. Cartesian coordinate and frequencies of structure **25** as in Figure S3

E= -308.683036404 Hartree

C	0.39350100	1.23949000	-0.00001400
C	-0.62644100	0.19830100	-0.00000400
C	0.15562200	-0.87955500	-0.00000700
C	1.38003100	-1.39943200	-0.00000200
C	2.27666400	-0.28841000	0.00001500
C	1.76330900	1.01045800	-0.00000100
H	-0.02499300	2.24491300	-0.00001300
H	1.68620400	-2.43869300	-0.00001200
H	3.33981000	-0.50977700	0.00001900
H	2.43958400	1.85808400	0.00000100
H	-4.04922600	-0.22375500	0.00002900
C	-2.06055200	0.46269800	0.00000700
C	-2.99882400	-0.49232600	-0.00000200
H	-2.32597500	1.51476400	0.00003400
H	-2.76526600	-1.55287300	-0.00001300

Frequencies --	86.7790	151.4512	173.3940
Frequencies --	336.2583	370.9892	426.8935
Frequencies --	467.4883	520.0011	538.2271
Frequencies --	675.9432	679.0519	759.0462
Frequencies --	787.9791	886.3685	904.9486
Frequencies --	973.3062	1000.5900	1002.9075

Frequencies --	1003.1733	1025.8362	1075.6155
Frequencies --	1130.7531	1188.6643	1239.6028
Frequencies --	1278.3244	1328.0868	1376.8297
Frequencies --	1458.1217	1496.0400	1506.1945
Frequencies --	1678.9288	1808.3129	3173.4566
Frequencies --	3175.2722	3212.2620	3212.5581
Frequencies --	3233.7571	3246.9385	3271.8612

Table S5. Cartesian coordinate and frequencies of structure **26** as in Figure S3

E= -308.738972908

C	-0.78691300	1.44438700	-0.00001300
C	0.45208800	0.74646400	0.00002400
C	0.54924800	-0.68429000	0.00000500
C	-0.56231600	-1.49202700	0.00002400
C	-1.78720300	-0.79155200	0.00001300
C	-1.90167200	0.62993400	-0.00001900
H	-0.85775900	2.52678200	-0.00002100
H	-0.53324900	-2.57579100	0.00003600
H	-2.70955500	-1.36669400	-0.00000500
H	-2.89530200	1.06446500	-0.00005300
C	1.82972300	0.88242100	0.00002500
C	2.09087500	-0.62859900	-0.00003900
H	2.59546700	-1.01366300	-0.89192500
H	2.50185300	1.73822700	0.00010900

H	2.59556900	-1.01375300	0.89174900

Frequencies --	83.6485	217.5156	374.2978
Frequencies --	430.2562	451.2882	546.1875
Frequencies --	644.5902	696.6290	776.1056
Frequencies --	786.0377	882.2927	898.5848
Frequencies --	905.2131	909.2248	1002.2733
Frequencies --	1008.2498	1042.8707	1051.1992
Frequencies --	1110.9945	1145.8422	1155.8509
Frequencies --	1198.0558	1236.1913	1258.3584
Frequencies --	1287.6650	1379.5020	1443.3907
Frequencies --	1462.4326	1483.2646	1538.8975
Frequencies --	1645.8736	1652.9041	3076.8544
Frequencies --	3127.8174	3204.7851	3213.1126
Frequencies --	3224.2445	3233.8749	3235.9609

Table S6. Cartesian coordinate and frequencies of structure **S2** as in Figure S4

E= -307.411735473 Hartree

C	0.11385800	1.14778500	-0.00001100
C	-0.69512600	-0.06713600	0.00000800
C	0.26376000	-1.00377900	-0.00000300
C	1.56130600	-1.28661400	-0.00000900
C	2.23710700	-0.02741100	0.00001400
C	1.50163300	1.15990300	0.00000000

H	-0.48452800	2.05645200	-0.00001800
H	2.05562700	-2.25126400	-0.00002100
H	3.32310000	-0.05467300	0.00001800
H	2.01873300	2.11323100	-0.00000300
H	-4.37652100	-0.12750000	-0.00000300
C	-2.09866900	-0.10099800	0.00000500
C	-3.30660500	-0.11112500	0.00000100

Frequencies --	110.3973	141.0211	324.3043
Frequencies --	345.7184	363.2723	434.9836
Frequencies --	470.8894	520.1684	614.8278
Frequencies --	664.2307	709.9317	728.9103
Frequencies --	735.1134	777.9715	883.0858
Frequencies --	907.9001	972.7641	1001.3087
Frequencies --	1022.1337	1128.6130	1184.2995
Frequencies --	1243.8583	1277.2313	1355.5725
Frequencies --	1494.4567	1505.3123	1806.5859
Frequencies --	2245.0230	3188.0517	3209.1750
Frequencies --	3232.5115	3243.1207	3455.0918

Table S7. Cartesian coordinate and frequencies of structure **S3** as in Figure S4

E= -307.391443455 Hartree

C	-0.65003200	-1.47283700	-0.00001300
C	0.55028800	-0.78986300	-0.00026000

C	0.62950900	0.65899300	-0.00021600
C	-0.50503100	1.48769900	-0.00013200
C	-1.70946100	0.79169100	0.00004400
C	-1.77895500	-0.63701100	0.00022400
H	-0.73169800	-2.55434600	-0.00013000
H	-0.45875400	2.57137200	-0.00014200
H	-2.64465400	1.34275600	0.00015200
H	-2.76703000	-1.08889100	0.00015200
H	2.85108000	1.31162700	0.00056800
C	2.04188200	-0.88308400	0.00003400
C	2.04697500	0.58065700	0.00021900

Frequencies -- 175.5758 291.4921 374.2799

Frequencies -- 442.3494 535.2836 556.5833

Frequencies -- 584.4560 765.7382 791.0467

Frequencies -- 824.2127 877.5669 913.8889

Frequencies -- 961.0874 992.4041 999.0133

Frequencies -- 1044.2860 1049.1419 1120.2373

Frequencies -- 1153.1747 1191.3511 1217.9918

Frequencies -- 1246.0893 1322.3153 1426.9236

Frequencies -- 1466.7115 1503.3419 1565.0406

Frequencies -- 1623.8618 3210.4475 3221.6380

Frequencies -- 3233.1166 3234.3046 3235.1469

Table S8. Cartesian coordinate and frequencies of structure **S4** as in Figure S5

E= -417.001411838 Hartree

C	-0.95198600	-1.52943700	0.00003000
C	0.19447300	-0.72094700	0.00000200
C	-0.04245100	0.68778300	-0.00000300
C	-1.32509300	1.27657100	-0.00000600
C	-2.41790000	0.42948300	0.00001700
C	-2.22623500	-0.96339300	0.00003600
H	-0.82535200	-2.60578000	0.00004700
H	-1.43349700	2.35538100	-0.00001600
H	-3.41925800	0.84467000	0.00002400
H	-3.09178200	-1.61811700	0.00005500
N	1.04824800	1.51275700	-0.00001400
N	1.94852800	2.17326600	-0.00008200
H	3.61454300	-2.11687500	0.00001800
C	1.50527600	-1.25081900	0.00000400
C	2.62690300	-1.70614700	0.00001000

Frequencies --	110.7953	114.4787	166.8912
Frequencies --	192.4548	357.4884	391.6776
Frequencies --	414.6391	457.6657	533.5275
Frequencies --	557.2795	571.2965	607.9312
Frequencies --	707.8708	713.7249	721.9210
Frequencies --	728.1055	779.8819	821.2772

Frequencies --	903.9459	989.8824	1034.3472
Frequencies --	1052.7685	1116.8584	1183.7865
Frequencies --	1207.4656	1234.5103	1302.9861
Frequencies --	1364.3814	1459.6600	1506.8327
Frequencies --	1584.9342	1624.1681	2222.9162
Frequencies --	2338.0647	3217.5970	3227.3611
Frequencies --	3236.0336	3239.3820	3456.9085

Table S8. Cartesian coordinate and frequencies of structure **21** as in Figure S5

E= -416.976217453 Hartree

C	1.18734200	1.46046600	0.00005900
C	-0.05052600	0.77959400	0.00003500
C	-0.01857200	-0.70721700	-0.00002500
C	1.20369900	-1.39602200	-0.00004800
C	2.37968700	-0.67163700	-0.00001700
C	2.36743900	0.74253400	0.00003600
H	1.18716800	2.54380300	0.00010000
H	1.19371800	-2.48025300	-0.00009000
H	3.32937100	-1.19542600	-0.00003300
H	3.31034200	1.27920100	0.00006100
N	-1.23295000	-1.30277900	-0.00007700
N	-2.30082900	-0.72261400	-0.00005500
H	-3.55124100	1.03270600	0.00005500
C	-1.33186000	1.26079900	0.00006200

C	-2.52602500	0.69777100	0.00003700

Frequencies --	171.2435	203.8565	368.4679
Frequencies --	398.7782	457.0994	458.7186
Frequencies --	511.9656	562.6976	568.3632
Frequencies --	584.4039	656.1012	704.2106
Frequencies --	707.7491	785.7744	786.3561
Frequencies --	793.9982	845.8295	882.5851
Frequencies --	996.1858	1029.7038	1035.6773
Frequencies --	1097.8114	1143.2606	1191.2236
Frequencies --	1219.5419	1256.0810	1329.5705
Frequencies --	1340.2555	1436.1843	1480.6539
Frequencies --	1552.4758	1620.1548	1647.7200
Frequencies --	1777.2297	3219.7959	3227.6788
Frequencies --	3236.2065	3240.8152	3313.4813

Table S9. Cartesian coordinate and frequencies of tolyl cation in Figure 5

E= -270.603002583 Hartree

C	-1.26655200	-1.26434200	0.00043700
C	0.03903200	-0.99812500	-0.00161900
C	1.01480000	-0.10039800	0.00068800
C	0.24076500	1.12618100	-0.00013900
C	-1.14952600	1.17756600	-0.00018100
C	-1.91209400	0.00781500	0.00005400

H	-1.77888600	-2.21878100	0.00192000
H	0.85247900	2.02695700	0.00012500
H	-1.64287500	2.14315800	0.00028600
H	-2.99841900	0.00832400	0.00066700
C	2.51696200	-0.17720400	0.00030700
H	2.93412700	0.82978100	0.00864600
H	2.86687600	-0.71681600	0.88405700
H	2.86637100	-0.70158400	-0.89298300

Frequencies --	45.0387	168.9284	284.1908
Frequencies --	378.3347	394.5149	451.3067
Frequencies --	532.4227	594.9254	673.9633
Frequencies --	755.7913	762.5237	887.1375
Frequencies --	908.5723	976.9216	978.2079
Frequencies --	1014.9528	1054.4505	1105.9883
Frequencies --	1131.4055	1191.0025	1230.1302
Frequencies --	1286.9831	1362.2549	1415.1125
Frequencies --	1481.8064	1487.0956	1496.9165
Frequencies --	1506.3009	1814.2466	3073.2864
Frequencies --	3149.9727	3176.0696	3178.6459
Frequencies --	3209.2759	3234.3692	3249.9359

Table S10. Cartesian coordinate and frequencies of benzyl cation in Figure 5

E= -270.672868600 Hartree

C	-1.12126700	1.23564400	0.00013200
C	0.25419100	1.24636900	-0.00044500
C	0.98274400	0.00006800	-0.00025300
C	0.25434700	-1.24633400	-0.00032900
C	-1.12114200	-1.23568700	-0.00009500
C	-1.80195200	-0.00006300	0.00031700
H	-1.68392200	2.16245400	0.00040600
H	0.80765400	-2.18058400	-0.00023700
H	-1.68378400	-2.16251900	-0.00007500
H	-2.88865400	-0.00016300	0.00079100
C	2.35286100	0.00005900	0.00038900
H	2.92145300	0.92664900	0.00033400
H	2.92110200	-0.92677600	0.00120000
H	0.80746500	2.18059600	-0.00072000

Frequencies --	166.1988	341.9459	360.2014
Frequencies --	419.1449	534.5587	610.0378
Frequencies --	629.2352	644.6944	800.7248
Frequencies --	824.4590	851.2235	987.3037
Frequencies --	1002.1199	1002.6597	1016.6352
Frequencies --	1026.3744	1052.9073	1105.3651
Frequencies --	1138.5665	1205.5362	1215.5097
Frequencies --	1356.3967	1390.8512	1430.5612
Frequencies --	1484.9764	1506.4458	1582.6172

Frequencies --	1604.9927	1673.5565	3164.9305
Frequencies --	3208.5317	3213.4582	3215.3176
Frequencies --	3232.7475	3235.3785	3266.5332

Table S11. Cartesian coordinate and frequencies corresponding to the transition state TS2 as in Figure 5

E= -270.561135164; Imaginary frequency: -632.7696 cm^{-1}

C	-0.65047800	-1.47776200	-0.03740000
C	0.50259300	-0.77400900	0.16603200
C	0.85423700	0.49988800	0.10747300
C	-0.14985000	1.46299100	0.01787400
C	-1.43668600	0.89957000	-0.02253000
C	-1.67065800	-0.49328000	-0.03811700
H	-0.81448400	-2.54536900	-0.07084700
H	0.02502800	2.52995700	-0.04796000
H	-2.29853800	1.55689500	-0.07116900
H	-2.69453700	-0.85823900	-0.03288100
C	2.24874000	-0.04433200	-0.09600500
H	2.69385100	0.08702400	-1.08451600
H	2.92126100	0.01703400	0.76292300
H	1.98003200	-1.22569700	-0.03951100

Frequencies --	-632.7696	120.2278	343.5120
Frequencies --	400.5666	462.8201	538.5044
Frequencies --	602.6885	622.9806	688.6694

```
Frequencies --   728.7879     846.5501     870.9897

Frequencies --   937.4300     948.8032     990.6710

Frequencies --  1006.0275    1011.4046    1128.7836

Frequencies --  1167.3516    1204.2568    1235.8668

Frequencies --  1288.7134    1298.6265    1395.6718

Frequencies --  1444.9813    1472.7274    1495.1763

Frequencies --  1547.1183    1813.6086    2240.1402

Frequencies --  3084.0350    3198.5178    3199.1371

Frequencies --  3224.1336    3247.9843    3278.7634
```