Reference 3.
Gaussian 03, Revision B.04,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

C12H3+

C12H3+

B3LYP/6-31+G

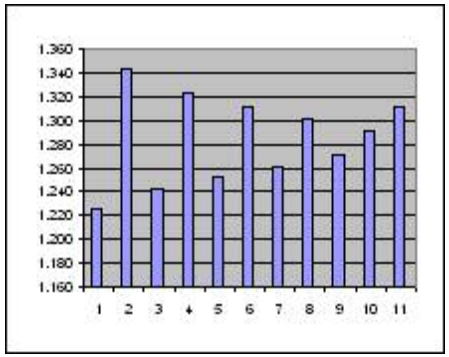
C12H2-Hcation-B3LYPs-SCFp

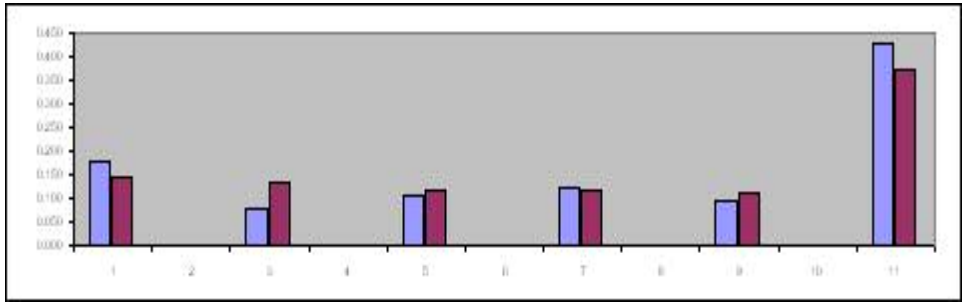
E = -458.3918326

	R(1,2)	R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)
	1.226	1.344	1.242	1.324	1.252	1.312	1.261	1.301	1.271
	C1	C2	C3	C4	C5	C6	C7	C8	C9
ChelpG	0.130	0.047	0.158	-0.082	0.215	-0.111	0.231	-0.111	0.246
NBO	0.299	-0.154	0.173	-0.042	0.153	-0.034	0.151	-0.032	0.162
ChelpG		0.178		0.076		0.104		0.120	
NBO		0.145		0.131		0.119		0.119	

R(10,11)	R(11,12)
1.291	1.311

C10	C11	C12
-0.151	0.329	0.099
-0.050	0.192	0.183
0.095		0.428
0.112		0.375





C12H3+

B3LYP/6-31G

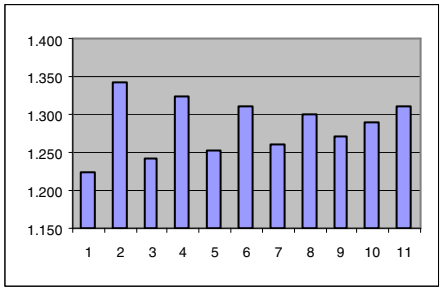
-458.3807179

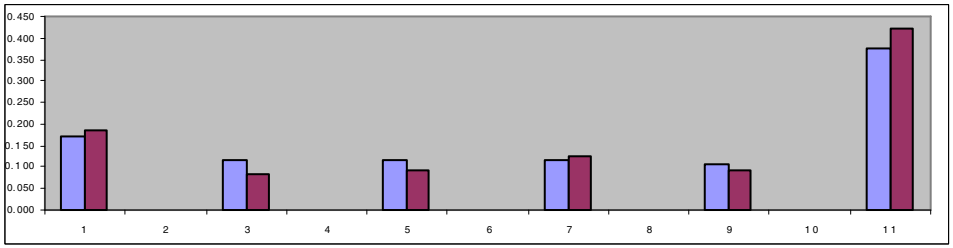
	R(1,2)	R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)
	1.225	1.343	1.242	1.323	1.252	1.311	1.261	1.301	1.271

	C1	C2	C3	C4	C5	C6	C7	C8	C9
NBO	0.304	-0.134	0.159	-0.042	0.147	-0.032	0.146	-0.030	0.156
CHELPG	0.133	0.054	0.137	-0.054	0.193	-0.101	0.224	-0.098	0.224
NBO		0.169		0.117		0.115		0.116	
CHELPG		0.187		0.083		0.092		0.126	

R(10,11)	R(11,12)
1.290	1.311

C10	C11	C12
-0.048	0.179	0.196
-0.132	0.304	0.116
0.107		0.376
0.092		0.420





3 S

C12H3+

B3LYP/6-31G*

C12H2-Hcation-B3LYPs-SCF

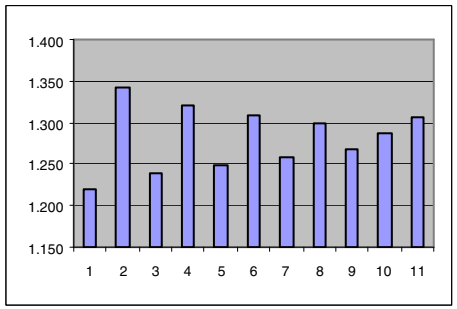
E = -458.4756506

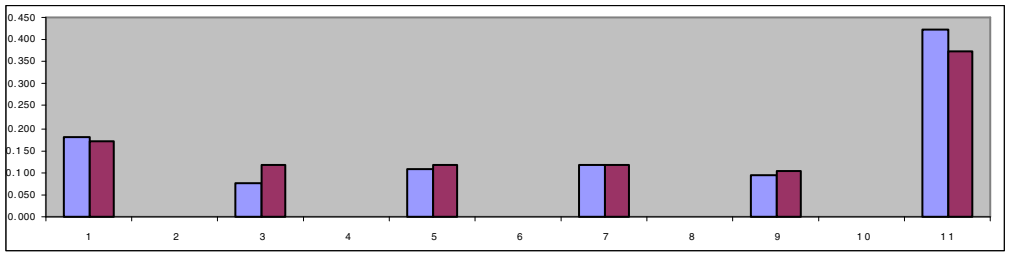
	R(1,2)	R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)
	1.219	1.342	1.238	1.322	1.249	1.309	1.258	1.299	1.268

	C1	C2	C3	C4	C5	C6	C7	C8	C9
ChelpG	0.140	0.041	0.168	-0.091	0.221	-0.112	0.232	-0.115	0.239
NBO	0.309	-0.138	0.164	-0.047	0.156	-0.039	0.153	-0.038	0.154
NBO		0.181		0.077		0.110		0.117	
CHELPG		0.171		0.116		0.117		0.116	

R(10,11)	R(11,12)
1.287	1.307

C10	C11	C12
-0.147	0.309	0.113
-0.050	0.175	0.200
0.092		0.423
0.104		0.375





4 S

C12H3+

HF/6-31G

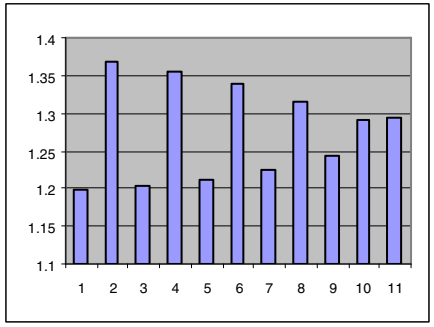
-455.4033173

	R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)	R(10,11)
	1.197	1.369	1.204	1.354	1.211	1.338	1.224	1.316	1.244

	C1	C2	C3	C4	C5	C6	C7	C8	C9
NBO	0.242	-0.162	0.169	-0.115	0.213	-0.135	0.259	-0.141	0.282

R(11,12)	R(12,13)
1.291	1.293

C10	C11	C12
-0.129	0.262	0.256

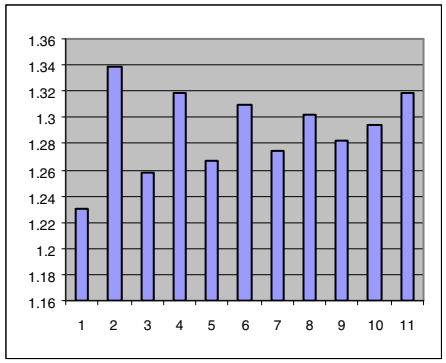


C12H3+

BPW91/6-31G		R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)	R(10,11)
-458.3633535		1.23	1.339	1.257	1.319	1.267	1.309	1.274	1.302	1.282
		C1	C2	C3	C4	C5	C6	C7	C8	C9
	NBO	0.316	-0.123	0.144	-0.019	0.123	-0.008	0.119	-0.007	0.130

R(11,12)	R(12,13)
1.295	1.319

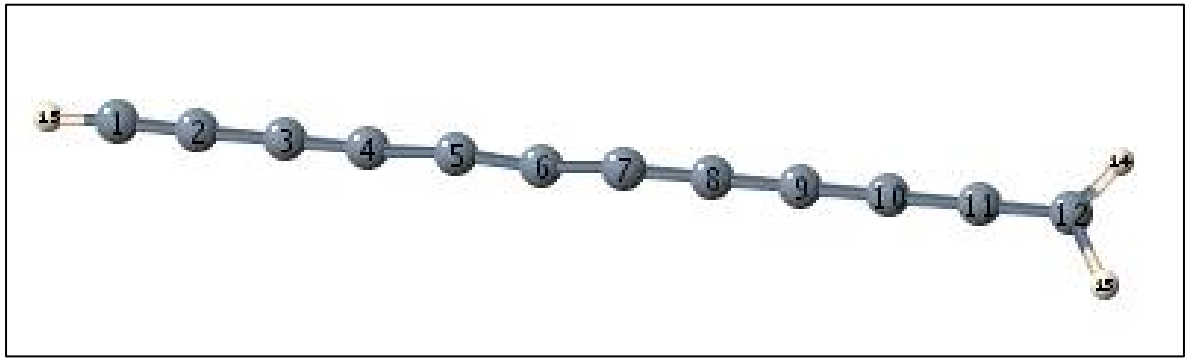
C10	C11	C12
-0.033	0.165	0.192

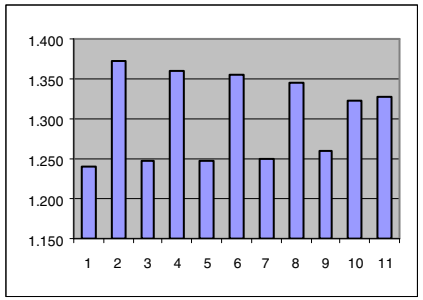


C12H3+

MP2/6-31G	R(1,2)	R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)
SCF=(QC, CONVER=5)	1.241	1.372	1.248	1.360	1.249	1.354	1.250	1.344	1.261
-456.455435									

Not perfectly linear. No neg. Freq





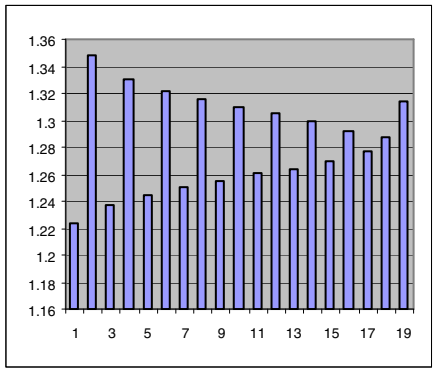
Equal contribution of all resonance structures in C12H3+

B3LYP/6-31G*											
C12H2-B3LYP	- 458.12	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11	C11-C12
		1.216	1.355	1.230	1.342	1.234	1.340	1.234	1.342	1.230	1.355	1.216
		1.222	1.356	1.233	1.344	1.237	1.341	1.237	1.344	1.233	1.356	1.281
		1.222	1.356	1.233	1.344	1.237	1.341	1.237	1.344	1.281	1.281	1.281
		1.222	1.356	1.233	1.344	1.237	1.341	1.281	1.281	1.281	1.281	1.281
		1.222	1.356	1.233	1.344	1.281	1.281	1.281	1.281	1.281	1.281	1.281
		1.222	1.356	1.281	1.281	1.281	1.281	1.281	1.281	1.281	1.281	1.281
		1.281	1.281	1.281	1.281	1.281	1.281	1.281	1.281	1.281	1.281	1.281
		7.390	8.061	7.496	7.937	7.554	7.867	7.599	7.812	7.640	7.762	7.687
		1.232	1.343	1.249	1.323	1.259	1.311	1.266	1.302	1.273	1.294	1.281

C20H3+

C20H3+										
B3LYP/6-31G		R(1,2)	R(2,3)	R(3,4)	R(4,5)	R(5,6)	R(6,7)	R(7,8)	R(8,9)	R(9,10)	R(10,11)
-762.974122		1.223	1.348	1.237	1.3311	1.245	1.322	1.2511	1.316	1.255	1.31
		H	C1	C2	C3	C4	C5	C6	C7	C8	C9
	NBO	0.268	-0.029	-0.126	0.109	-0.038	0.099	-0.030	0.097	-0.026	0.097
	CHELPG	0.260	-0.202	0.083	0.061	-0.023	0.114	-0.065	0.148	-0.089	0.171

R(11,12)	R(12,13)	R(13,14)	R(14,15)	R(15,16)	R(16,17)	R(17,18)	R(18,19)	R(19,20)				
1.2603	1.305	1.264	1.299	1.269	1.292	1.277	1.287	1.314				
C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	C20	H	H
-0.024	0.098	-0.022	0.100	-0.022	0.103	-0.024	0.115	-0.046	0.139	-0.411	0.286	0.286
-0.093	0.156	-0.065	0.134	-0.049	0.140	-0.073	0.187	-0.141	0.271	-0.343	0.209	0.209



C12H3. Radical geometry

B3LYP/6-31G

C12H2-Hradical-B3LYP	-458.63	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11	C11-C12
		1.224	1.352	1.240	1.332	1.252	1.319	1.263	1.305	1.278	1.290	1.321

C12H3+ CCSD(T)

C12H3+

CCSD(T)/6-31g*//B3LYP/6-31G*

-457.1339187

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
CHELPG	0.11666	-0.0004	0.227755	-0.20764	0.342642	-0.25701	0.366638	-0.22917	0.331925	-0.18226
NBO	0.30404	-0.1961	0.21129	-0.12976	0.2237	-0.12023	0.222	-0.09575	0.20654	-0.07244

C11	C12
0.305422	0.185428
0.17732	0.26937

C12H3+

B3LYP/6-31G*

-458.4547343

All C-C fixed to 1.3 A

	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3

	C1	C2	C3	C4	C5	C6	C7	C8	C9
CHELPG	0.188163	0.01946	0.170962	-0.07442	0.184949	-0.06972	0.177694	-0.07463	0.200394
NBO	0.3474	-0.13635	0.14656	-0.02138	0.12368	-0.01218	0.1172	-0.01003	0.12155

C10-C11	C11-C12
1.3	1.3

C10	C11	C12
-0.11858	0.267104	0.128635
-0.02411	0.14431	0.20335

C12H3+

b3lyp/6-31g*

-458.461

All bond opt. with the same length

C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11
1.2796	1.2796	1.2796	1.2796	1.2796	1.2796	1.2796	1.2796	1.2796	1.2796

	C1	C2	C3	C4	C5	C6	C7	C8	C9
CHELPG	0.184826	0.024482	0.16282	-0.0609	0.17208	-0.06103	0.171017	-0.06312	0.184992
NBO	0.34945	-0.14019	0.14815	-0.02239	0.12526	-0.01349	0.11903	-0.01166	0.12371

C11-C12
1.2796

C10	C11	C12
-0.10605	0.26449	0.126396
-0.0254	0.14354	0.204

C12H3+

ccsd(T)/6-31g*//B3LYP/6-31G*

-457.115559

All C-C fixed to 1.3 A

C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3

	C1	C2	C3	C4	C5	C6	C7	C8
CHELPG	0.200627	-0.05437	0.244489	-0.16193	0.246088	-0.11982	0.197858	-0.07535
NBO	0.36103	-0.19418	0.18182	-0.06395	0.13889	-0.02566	0.11254	-0.00094

C10-C11	C11-C12
1.3	1.3

C9	C10	C11	C12
0.178754	-0.07102	0.199392	0.215275
0.10399	0.00018	0.11258	0.27371

C12H3+

ccsd(T)/6-31g*//B3LYP/6-31G*

-457.1156875

All bond opt. with the same length

C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
1.27964	1.27964	1.27964	1.27964	1.27964	1.27964	1.27964	1.27964	1.27964

	C1	C2	C3	C4	C5	C6	C7	C8
CHELPG	0.197896	-0.04635	0.234718	-0.14637	0.233911	-0.11375	0.195865	-0.06766
NBO	0.36543	-0.19912	0.18701	-0.06819	0.14518	-0.03102	0.11853	-0.00613

C10-C11	C11-C12
1.27964	1.27964

C9	C10	C11	C12
0.165677	-0.06177	0.202936	0.204897
0.10893	-0.00377	0.11308	0.27008

C12H3+

B3LYP/6-31G*

-458.4704697

C1-C10 fixed from the neutral

C11-C12 opt in b3lyp/6-31G*

	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
	1.2163	1.355	1.2295	1.3425	1.2336	1.3399	1.2336	1.3425	1.2295

	C1	C2	C3	C4	C5	C6	C7	C8	C9
CHELPG	0.12237	0.050825	0.143633	-0.07379	0.196254	-0.10652	0.234026	-0.13348	0.283969
NBO	0.2945	-0.1362	0.15134	-0.04583	0.14397	-0.03829	0.14915	-0.04052	0.18408

C10-C11	C11-C12
1.296	1.3022

C10	C11	C12
-0.18132	0.359005	0.105024
-0.07644	0.21468	0.19955

C12H3+

ccsd(t)/6-31G*//B3LYP/6-31G*

-457.1309955

C1-C10 fixed from the neutral

C11-C12 opt in b3lyp/6-31G*

	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11
	1.2163	1.355	1.2295	1.3425	1.2336	1.3399	1.2336	1.3425	1.2295	1.296

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
CHELPG	0.080461	0.02965	0.177488	-0.17696	0.310902	-0.26334	0.399251	-0.30448	0.453447	-0.29328
NBO	0.27505	-0.18418	0.18526	-0.12617	0.21421	-0.1374	0.24666	-0.14211	0.2882	-0.14577

C11-C12

1.302

C11	C12
0.430856	0.156001
0.2645	0.26173

C11H3_ Anion

C12H3-

B3LYP/6-31G

-458.7029756

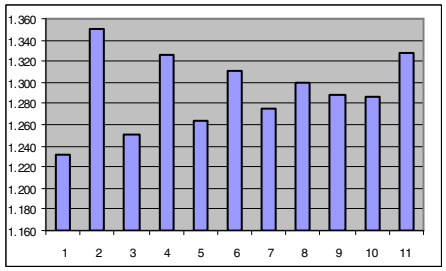
C12H2-Hanion-B3LYP

	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
	1.231	1.350	1.250	1.326	1.264	1.311	1.276	1.299	1.289

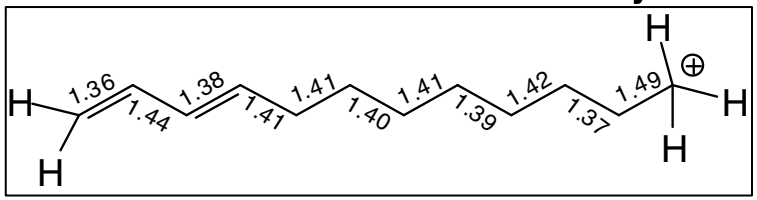
	C1	C2	C3	C4	C5	C6	C7	C8	C9
ChelpG	-0.2486	0.1333	-0.1792	-0.0133	-0.0872	-0.0867	-0.0589	-0.0892	-0.0538
NBO	-0.0636	-0.0869	-0.1298	-0.014	-0.1368	-0.0158	-0.1328	-0.0305	-0.1147

C10-C11	C11-C12
1.287	1.328

C10	C11	C12
-0.1587	0.04281	-0.2004
-0.076	-0.0764	-0.1227



C12H15+ Polyene



B3LYP/6-31G

			C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
C12H14-H-B3LYP	-465.92		1.355	1.435	1.378	1.414	1.414	1.400	1.405	1.386	1.424
			C1	C2	C3	C4	C5	C6	C7	C8	C9
		Mulliken	0.10244	0.09664	0.09045	0.05415	0.0893	0.05336	0.08952	0.05155	0.0926
		ChelpG	0.1209	0.04756	0.16228	-0.0195	0.14297	0.0143	0.13744	-0.0167	0.1798
		NBO	0.1975	-0.0264	0.14711	-0.0051	0.14776	-0.0039	0.14969	-0.0088	0.1585
				0.17109		0.14204		0.14391		0.1409	

C10-C11	C11-C12	
1.366	1.487	
C10	C11	C12
0.07102	0.11962	0.08935
-0.0528	0.16895	0.11479
-0.0344	0.20193	0.07601
0.12411		0.27794

C12H14-B3LYPs	-465.62		C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
neutral			1.345	1.446	1.358	1.437	1.361	1.435	1.361	1.437	1.358

C10-C11	C11-C12
1.446	1.345

C12H14-H-B3LYPs	-466.02		C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
Cation fully opt.			1.351	1.433	1.375	1.411	1.389	1.397	1.403	1.383	1.422
			C1	C2	C3	C4	C5	C6	C7	C8	C9
		CHELPG	0.11837	0.05204	0.15969	-0.0104	0.133	0.01662	0.12502	0.01758	0.14496
		NBO	0.20202	-0.0309	0.15086	-0.0099	0.15218	-0.0089	0.15427	-0.0139	0.16299
		CHELPG		0.17041		0.14929		0.14962		0.1426	
		NBO		0.17113		0.14093		0.14327		0.14034	

C10-C11	C11-C12	
1.362	1.485	
C10	C11	C12
-0.0457	0.1876	0.10125
-0.039	0.20331	0.07703
0.09923		0.28885
0.12399		0.28034

C12H14-B3LYPsF-C11-C12H3Free -466

Geometry of the neutral

		C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
		1.345	1.446	1.358	1.437	1.362	1.435	1.362	1.437	1.358
		C1	C2	C3	C4	C5	C6	C7	C8	C9
	CHELPG	0.0878	0.06432	0.13342	-0.0281	0.14538	0.00231	0.11363	0.01362	0.16986
	NBO	0.1766	-0.0315	0.12805	-0.0087	0.13221	-0.0054	0.13988	-0.0082	0.16021
	CHELPG		0.15212		0.10532		0.14769		0.12724	
	NBO		0.14508		0.11934		0.12678		0.13171	

C10-C11	C11-C12	
1.446	1.476	
C10	C11	C12
-0.0578	0.22429	0.13124
-0.0351	0.26234	0.08965
0.1121		0.35553
0.1251		0.35199

C12H14-B3LYPs-RCC-C11-C12H3Free	-466.01		C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
All resonating bonds identical			1.392	1.392	1.392	1.392	1.392	1.392	1.392	1.392	1.392
			C1	C2	C3	C4	C5	C6	C7	C8	C9
		CHELPG	0.13677	0.05013	0.1536	-0.0158	0.13537	0.02076	0.09833	0.02834	0.14178
		NBO	0.22076	-0.0304	0.14036	-0.0019	0.13619	-0.0027	0.1378	-0.0078	0.15013
		CHELPG		0.1869		0.13777		0.15612		0.12667	
		NBO		0.19034		0.13844		0.13346		0.13004	

C10-C11	C11-C12	
1.392	1.483	
C10	C11	C12
-0.0516	0.19826	0.10412
-0.0378	0.21735	0.07802
0.09015		0.30238
0.11233		0.29537

# Equal contribution of all resonance structures in C12H15+

B3LYP/6-31G*

C12H14-B3LYPs		-465.62	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
			1.345	1.446	1.358	1.437	1.361	1.435	1.361	1.437	1.358
			1.345	1.446	1.358	1.437	1.361	1.435	1.361	1.437	1.358
			1.345	1.446	1.358	1.437	1.361	1.435	1.361	1.437	1.440
			1.345	1.446	1.358	1.437	1.361	1.435	1.440	1.355	1.440
			1.345	1.446	1.358	1.437	1.440	1.355	1.440	1.355	1.440
			1.345	1.446	1.440	1.355	1.440	1.355	1.440	1.355	1.440
			1.440	1.446	1.440	1.355	1.440	1.355	1.440	1.355	1.440
			8.164	8.678	8.312	8.456	8.404	8.369	8.483	8.293	8.558
			1.361	1.446	1.385	1.409	1.401	1.395	1.414	1.382	1.426

		Aver single	
		Aver Double	
C10-C11	C11-C12		
1.446	1.345		1.394
1.446	1.485	**a**	
1.355	1.485	**b**	
1.355	1.485	**c**	
1.355	1.485	**d**	
1.355	1.485	**e**	
1.355	1.485	**f**	
8.221	8.910		
1.370	1.485		

C6H3+

C6H3+

B3LYP/6-31G*
C6H2-H-B3LYP-NBO
E=-229.9650992

	C(1,2)	C(2,3)	C(3,4)	C(4,5)	C(5,6)	
	1.224	1.331	1.250	1.302	1.297	
	C1	C2	C3	C4	C5	C6
NBO	0.43375	-0.15594	0.2648	-0.07134	0.26953	0.25919
CHELPG	-0.13112	0.429952	-0.16403	0.300047	0.003331	0.561814
		0.27781		0.19346		0.52872

All C-C bonds are equal
C6H3-R1-B3LYP-NBO-CHELPG
E=-229.9562194

	C(1,2)	C(2,3)	C(3,4)	C(4,5)	C(5,6)	
	1.279	1.279	1.279	1.279	1.279	
	C1	C2	C3	C4	C5	C6
NBO	0.46244	-0.15045	0.23248	-0.03879	0.22733	0.26699
CHELPG	0.307434	-0.01068	0.292935	-0.14964	0.392983	0.166971

C-C bonds from the neutral
C6H3-R1-R6F-B3LYP-NBO-CHELPG
E=-229.9518849

	C(1,2)	C(2,3)	C(3,4)	C(4,5)	C(5,6)	
	1.215	1.360	1.223	1.360	1.215	
	C1	C2	C3	C4	C5	C6
NBO	0.40603	-0.14943	0.25055	-0.0735	0.31118	0.25517
CHELPG	0.251578	-0.00065	0.308968	-0.20021	0.505049	0.135262

C40H3

B3LYP/6-31G*
C40H3-B3LYPs
E=-1524.7498314

	C(1,2)	C(2,3)	C(3,4)	C(4,5)	C(5,6)	C(6,7)	C(7,8)	C(8,9)	C(9,10)	C(10,11)
	1.217	1.352	1.232	1.337	1.238	1.330	1.241	1.327	1.239	1.324

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
NBO	0.18638	-0.12261	0.06337	-0.03437	0.05278	-0.02642	0.05049	-0.02346	0.051	-0.02236
CHELPG	0.001522	0.090589 0.06377	0.010975	-0.01678 0.029	0.054886	-0.03362 0.02636	0.063119	-0.04059 0.02703	0.080823	-0.06074 0.02864

C40H3-R1

C(11,12)	C(12,13)	C(13,14)	C(14,15)	C(15,16)	C(16,17)	C(17,18)	C(18,19)	C(19,20)	C(20,21)	C(21,22)	C(22,23)	C(23,24)
1.245	1.321	1.247	1.319	1.248	1.317	1.250	1.315	1.251	1.313	1.253	1.311	1.255

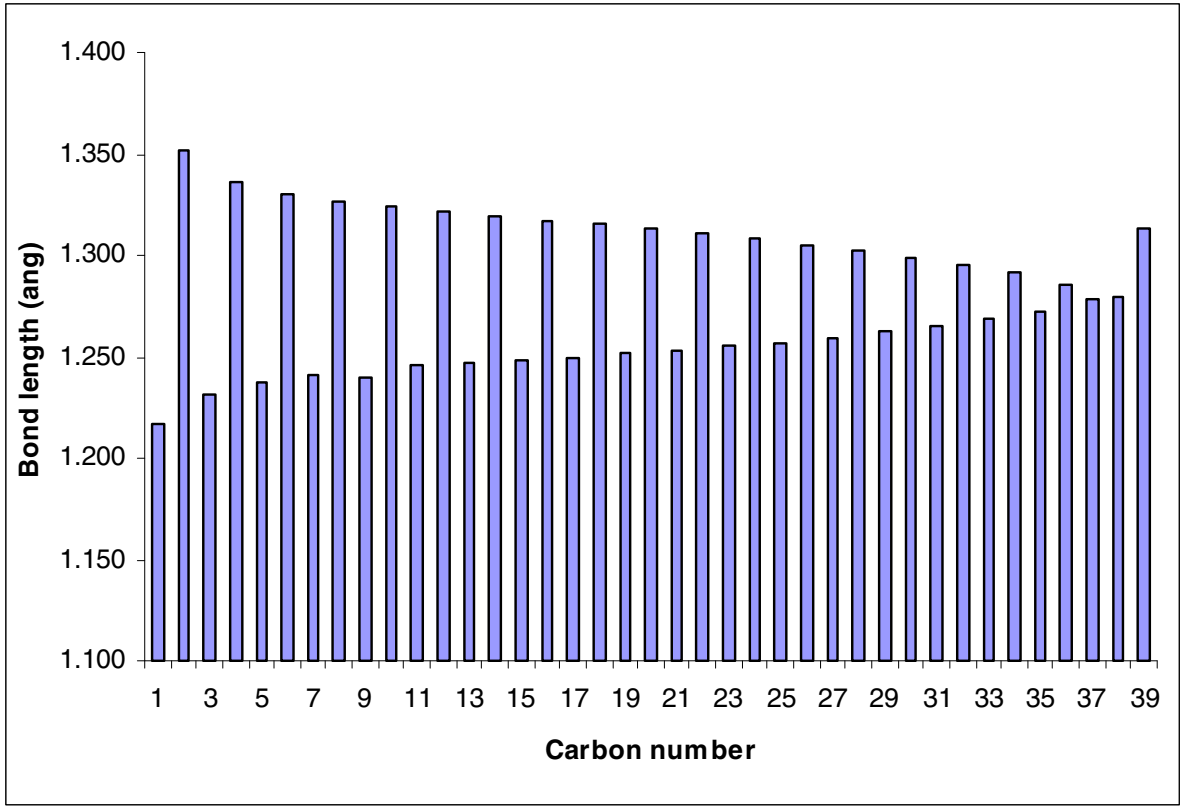
C11	C12	C13	C14	C15	C16	C17	C18	C19	C20	C21	C22	C23
-0.05236	-0.02188	0.05414	-0.02174	0.0561	-0.0217	0.05812	-0.02167	0.06008	-0.02155	0.06197	-0.0214	0.06377
-0.097875	-0.06605 0.03048	0.096573	-0.06089 0.0324	0.087271	-0.04036 0.0344	0.071254	-0.03431 0.03645	0.071272	-0.02496 0.03853	0.061684	-0.02133 0.04057	0.065567

C(24,25)	C(25,26)	C(26,27)	C(27,28)	C(28,29)	C(29,30)	C(30,31)	C(31,32)	C(32,33)	C(33,34)	C(34,35)	C(35,36)	C(36,37)
1.308	1.257	1.305	1.259	1.302	1.262	1.299	1.265	1.295	1.269	1.291	1.273	1.286

C24	C25	C26	C27	C28	C29	C30	C31	C32	C33	C34	C35	C36
-0.02114	0.0654	-0.02077	0.06686	-0.0203	0.06813	-0.0198	0.06942	-0.01955	0.07098	-0.02012	0.07407	-0.02397
-0.02287	0.07304	-0.03888	0.103698	-0.06829	0.123144	-0.07677	0.13077	-0.08272	0.133363	-0.08043	0.142104	-0.10127
0.04263		0.04463		0.04656		0.04833		0.04987		0.05086		0.0501

C(37,38)	C(38,39)	C(39,40)
1.279	1.280	1.314

C37	C38	C39
0.08462	-0.04721	0.10708
-0.169339	-0.13718	0.22173
	0.03741	



Bond length distribution for $C_{40}H_3^+$ calculated a B3LYP/6-31+G*