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

Electronic Supplementary Information to:

Triphenylboroxine stability under low energy electron interactions

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1. Parent cation ion signal mass spectrum at 70 eV electron energy

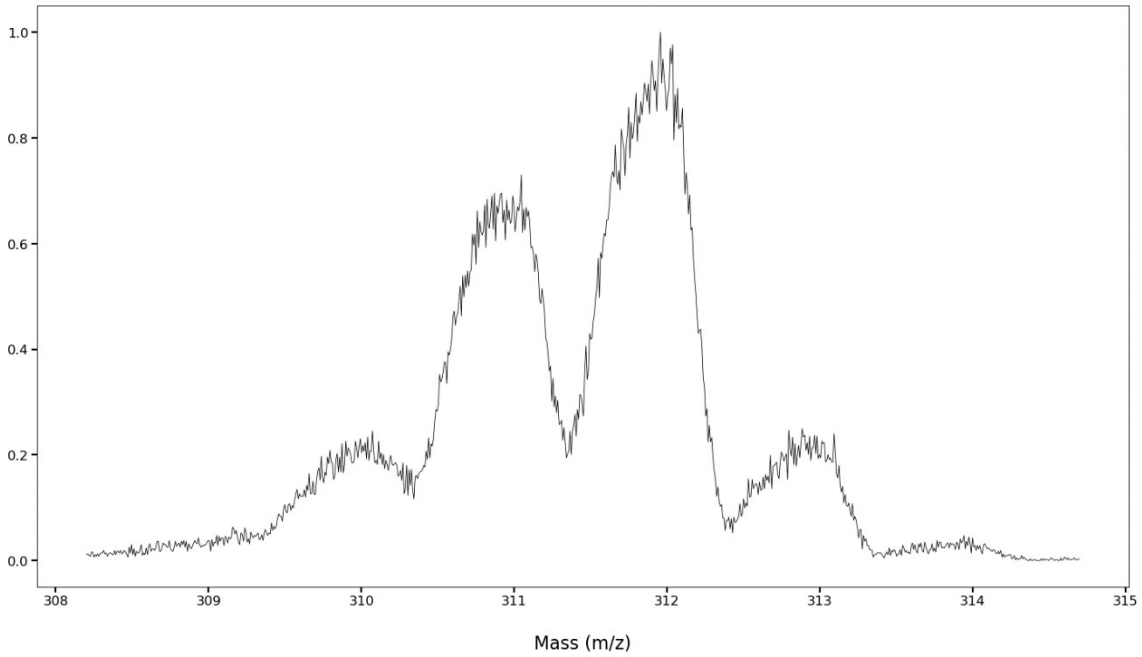
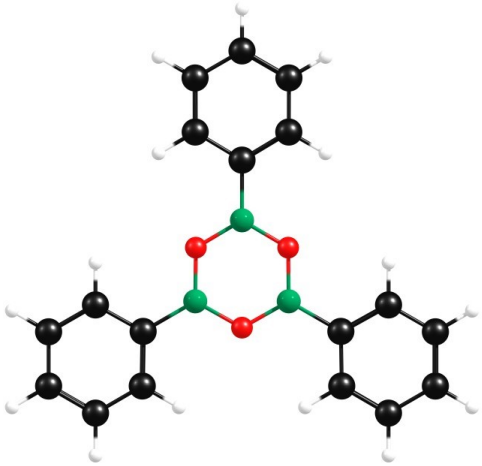


Figure S1. Parent cation ($(C_6H_6)_3O_3B_3^+$) mass spectrum recorded at 70 eV. Considering the parent cation at 312 m/z, the areas of the remaining peaks fragments are in agreement with the isotope distribution of the elements: 310 m/z (0.16), 311 m/z (0.67), 313 m/z (0.19), and 314 m/z (0.02).

2. G4(MP2) geometries

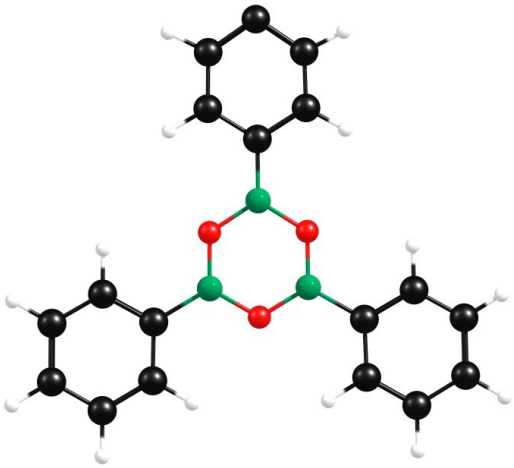
Tab S1: G4(MP2) geometry of the neutral triphenylboroxine molecule. Coordinates in angstroms.



	x	y	z
C	4.996039461	1.485120466	0.000000000
C	4.995843052	2.884351331	0.000000000
C	3.785543536	0.789919803	0.000000000
C	2.553677437	1.474366356	0.000000000
C	2.576862381	2.883416968	0.000000000
C	3.784171781	3.584136859	0.000000000
H	5.942369141	3.430828416	0.000000000
H	5.942290506	0.938744649	0.000000000
H	3.786393738	-0.302491518	0.000000000
H	3.784121970	4.676802210	0.000000000
H	1.631231527	3.430358925	0.000000000
B	1.207476096	0.697136647	0.000000000
B	0.000000000	-1.394273295	0.000000000
B	-1.207476096	0.697136647	0.000000000

O	0.000000000	1.376996949	0.000000000
O	1.192514340	-0.688498474	0.000000000
O	-1.192514340	-0.688498474	0.000000000
C	-2.553677437	1.474366356	0.000000000
C	-2.576862381	2.883416968	0.000000000
C	-3.784171781	3.584136859	0.000000000
C	-4.995843052	2.884351331	0.000000000
C	-4.996039461	1.485120466	0.000000000
C	-3.785543536	0.789919803	0.000000000
H	-3.784121970	4.676802210	0.000000000
H	-1.631231527	3.430358925	0.000000000
H	-5.942290506	0.938744649	0.000000000
H	-5.942369141	3.430828416	0.000000000
H	-3.786393738	-0.302491518	0.000000000
C	0.000000000	-2.948732712	0.000000000
C	1.208681149	-3.673336765	0.000000000
C	1.211867680	-5.069257325	0.000000000
C	0.000000000	-5.768702640	0.000000000
C	-1.211867680	-5.069257325	0.000000000
C	-1.208681149	-3.673336765	0.000000000
H	2.155162206	-3.127867408	0.000000000
H	-2.155162206	-3.127867408	0.000000000
H	-2.158168541	-5.615546838	0.000000000
H	0.000000000	-6.861656811	0.000000000
H	2.158168541	-5.615546838	0.000000000

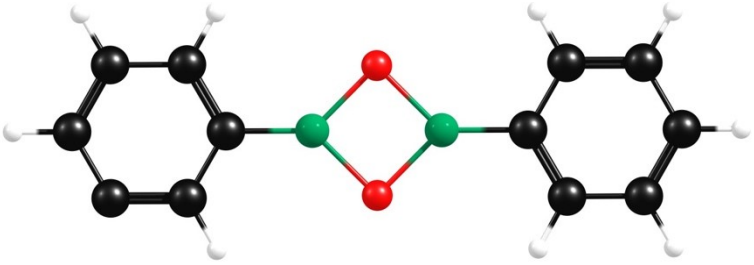
Tab S2: G4(MP2) geometry of the anionic fragment 311 m/z. Coordinates in angstroms.



	x	y	z
C	1.068710000	-5.133579000	-0.000207000
C	-0.124101000	-5.920664000	0.000267000
C	1.123444000	-3.747259000	-0.000407000
C	-0.059539000	-2.968570000	-0.000107000
C	-1.275295000	-3.695040000	0.000405000
C	-1.281357000	-5.082375000	0.000547000
H	2.036660000	-5.650898000	-0.000446000
H	2.085267000	-3.229847000	-0.000886000
H	-2.270992000	-5.556940000	0.000910000
H	-2.213324000	- 3.135721000	0.000780000
B	-0.028391000	-1.462158000	-0.000290000
B	1.207384000	0.629677000	-0.000622000
B	-1.178805000	0.677986000	0.000110000
O	-1.198777000	-0.677787000	0.000703000
O	1.172731000	-0.725816000	-0.001236000
O	0.028515000	1.357605000	-0.000208000
C	-2.515600000	1.491519000	0.000045000

C	-3.752729000	0.828699000	0.000363000
C	-4.950019000	1.537986000	0.000270000
C	-4.932696000	2.932022000	-0.000152000
C	-3.715288000	3.611017000	-0.000482000
C	-2.522147000	2.894302000	-0.000376000
H	-5.896824000	1.006325000	0.000508000
H	-3.760674000	-0.256473000	0.000676000
H	-3.698950000	4.697027000	-0.000813000
H	-5.865830000	3.488018000	-0.000233000
H	-1.573471000	3.421901000	-0.000626000
C	2.575485000	1.388999000	-0.000226000
C	3.785700000	0.678202000	-0.000353000
C	5.009802000	1.340188000	0.000065000
C	5.047209000	2.733833000	0.000626000
C	3.857346000	3.459990000	0.000762000
C	2.637116000	2.790467000	0.000338000
H	3.751444000	-0.406459000	-0.000778000
H	1.709699000	3.354612000	0.000449000
H	3.883542000	4.545806000	0.001200000
H	6.001435000	3.252787000	0.000960000
H	5.935084000	0.771880000	-0.000031000

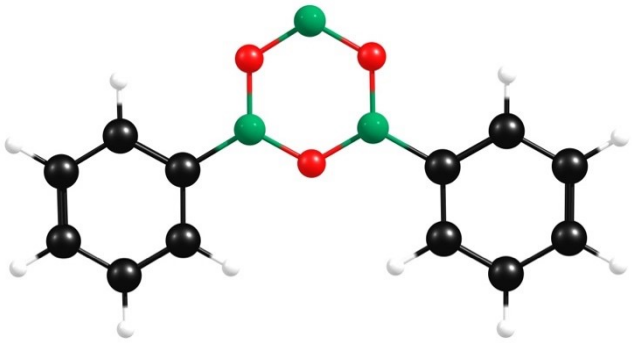
Tab S3: G4(MP2) geometry of the anionic fragment 207 m/z. Coordinates in angstroms.



	x	y	z
C	0.000000000	0.000000000	-5.536864000
C	-1.207444000	0.000000000	-4.840512000
C	-1.210118000	0.000000000	-3.446461000
C	1.207444000	0.000000000	-4.840512000
C	1.210118000	0.000000000	-3.446461000
C	0.000000000	0.000000000	-2.743426000
H	0.000000000	0.000000000	-6.615579000
H	2.152878000	0.000000000	-2.918866000
H	-2.152878000	0.000000000	-2.918866000
H	-2.141506000	0.000000000	-5.380924000
B	0.000000000	0.000000000	-1.175979000
B	0.000000000	0.000000000	1.175979000
O	-1.175976000	0.000000000	0.000000000
O	1.175976000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.743426000
C	1.210118000	0.000000000	3.446461000
C	1.207444000	0.000000000	4.840512000
C	0.000000000	0.000000000	5.536864000
C	-1.207444000	0.000000000	4.840512000
C	-1.210118000	0.000000000	3.446461000
H	2.152878000	0.000000000	2.918866000

H	0.000000000	0.000000000	6.615579000
H	2.141506000	0.000000000	5.380924000
H	-2.152878000	0.000000000	2.918866000
H	-2.141506000	0.000000000	5.380924000

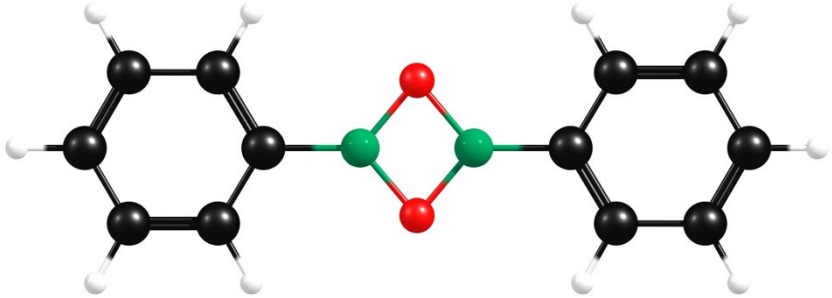
Tab S4: G4(MP2) geometry of the cationic fragment 235 m/z. Coordinates in angstroms.



	x	y	z
B	-0.000341000	2.894617000	-0.000069000
B	1.207766000	0.803628000	0.000035000
B	-1.207223000	0.802848000	-0.000027000
O	-1.192669000	2.188518000	-0.000073000
O	1.192391000	2.189211000	-0.000005000
O	0.000432000	0.123397000	0.000040000
C	-2.553398000	0.025569000	-0.000032000
C	-3.784922000	0.710629000	0.000146000
C	-4.995827000	0.016161000	0.000162000
C	-4.996461000	- 1.383049000	0.000005000
C	-3.785150000	-2.083473000	-0.000163000
C	-2.577406000	-1.383473000	-0.000193000
H	-5.941737000	0.563118000	0.000314000
H	-3.785163000	1.803035000	0.000298000
H	-3.785672000	-3.176143000	-0.000261000
H	-5.943262000	-1.929049000	0.000038000
H	-1.632179000	-1.931133000	-0.000308000
C	2.554089000	0.026626000	0.000021000
C	3.786178000	0.710690000	-0.000064000

C	4.996441000	0.015058000	-0.000059000
C	4.995724000	-1.384177000	0.000018000
C	3.783820000	-2.083552000	0.000107000
C	2.576758000	-1.382411000	0.000112000
H	3.787425000	1.803111000	-0.000125000
H	1.630892000	-1.928922000	0.000194000
H	3.783438000	-3.176216000	0.000186000
H	5.942060000	-1.930980000	0.000030000
H	5.942876000	0.561121000	-0.000114000

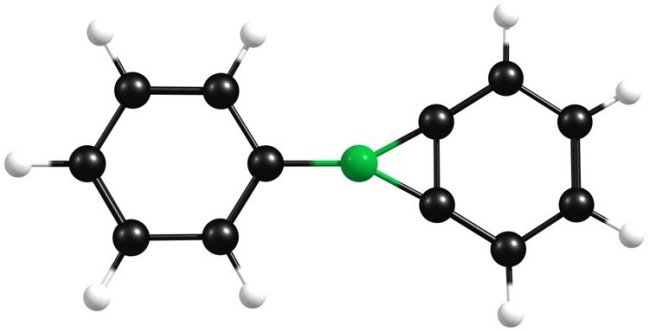
Tab S5: G4(MP2) geometry of the cationic fragment 208 m/z. Coordinates in angstroms.



	x	y	z
C	-0.000001000	0.000001000	-5.283534000
C	-1.201759000	0.000000000	-4.581927000
C	-1.200239000	0.000000000	-3.164485000
C	1.201758000	0.000000000	-4.581929000
C	1.200240000	0.000000000	-3.164487000
C	0.000001000	0.000000000	-2.443272000
H	2.146523000	0.000001000	-5.114113000
H	-0.000002000	0.000001000	-6.367198000
H	2.146508000	0.000000000	-2.633167000
H	-2.146506000	0.000000000	-2.633165000
H	-2.146524000	0.000001000	-5.114110000
B	0.000001000	-0.000001000	-0.903930000
B	0.000001000	-0.000001000	0.903930000
O	-1.073431000	-0.000002000	0.000000000
O	1.073434000	-0.000002000	0.000000000
C	0.000001000	0.000000000	2.443272000
C	1.200240000	0.000000000	3.164487000
C	1.201758000	0.000000000	4.581929000
C	-0.000001000	0.000001000	5.283534000
C	-1.201759000	0.000000000	4.581928000

C	-1.200239000	0.000000000	3.164485000
H	2.146508000	0.000000000	2.633167000
H	-0.000002000	0.000001000	6.367198000
H	2.146523000	0.000001000	5.114113000
H	-2.146506000	0.000000000	2.633165000
H	-2.146524000	0.000001000	5.114110000

Tab S6: G4(MP2) geometry of the cationic fragment 164 m/z. Coordinates in angstroms.



	x	y	z
C	0.000000000	0.000000000	4.164605000
C	0.000000000	1.198021000	3.458871000
C	0.000000000	-1.198021000	3.458871000
C	0.000000000	-1.194747000	2.034511000
C	0.000000000	0.000000000	1.303070000
C	0.000000000	1.194747000	2.034511000
H	0.000000000	2.145725000	3.986276000
H	0.000000000	0.000000000	5.248061000
H	0.000000000	-2.145302000	1.511205000
H	0.000000000	-2.145725000	3.986276000
H	0.000000000	2.145302000	1.511205000
C	0.000000000	-0.696970000	-1.540514000
C	0.000000000	0.696970000	-1.540514000
C	0.000000000	-1.442669000	-2.740412000
C	0.000000000	-0.704181000	-3.927173000
C	0.000000000	0.704181000	-3.927173000
C	0.000000000	1.442669000	-2.740412000
H	0.000000000	2.527492000	-2.764671000
H	0.000000000	-2.527492000	-2.764671000
H	0.000000000	-1.225427000	-4.878634000

H	0.000000000	1.225427000	-4.878634000
B	0.000000000	0.000000000	-0.237171000