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

Electronic Supplementary Information

$B_3@Si_{12}^+$: Strong stabilizing effects of triatomic cyclic boron unit on tubular silicon clusters

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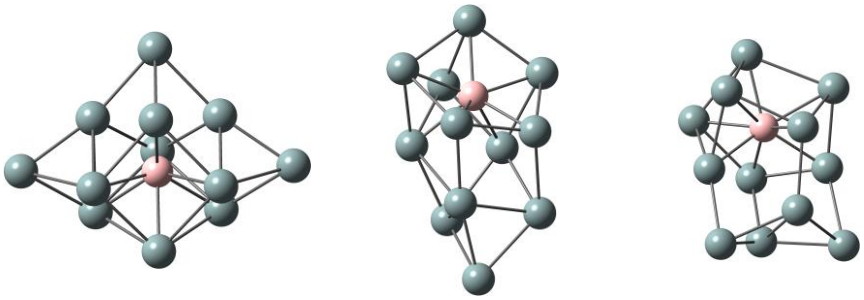
Table of content:

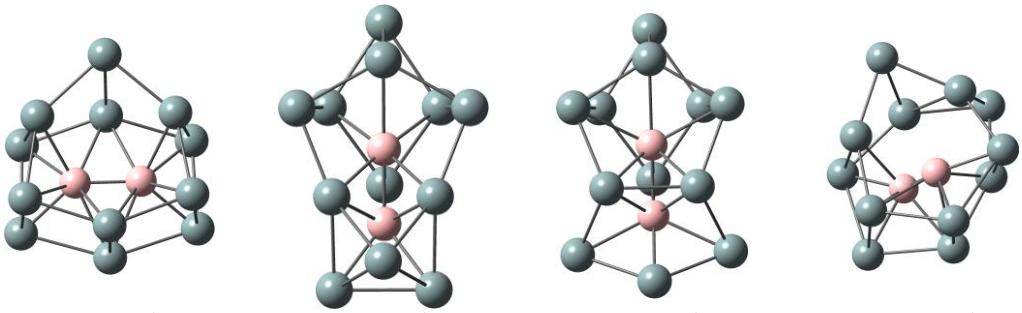


12c.1 (C_s, ^{1}A') 0.0 [0.0] (2.8) {0.0}

12c.2 (C_1, ^{1}A) 1.9 [2.1] (0.0) {0.2}

12c.3 (C_1, ^{1}A) 16.7 [8.5] (2.3) {7.3}

Figure S1.



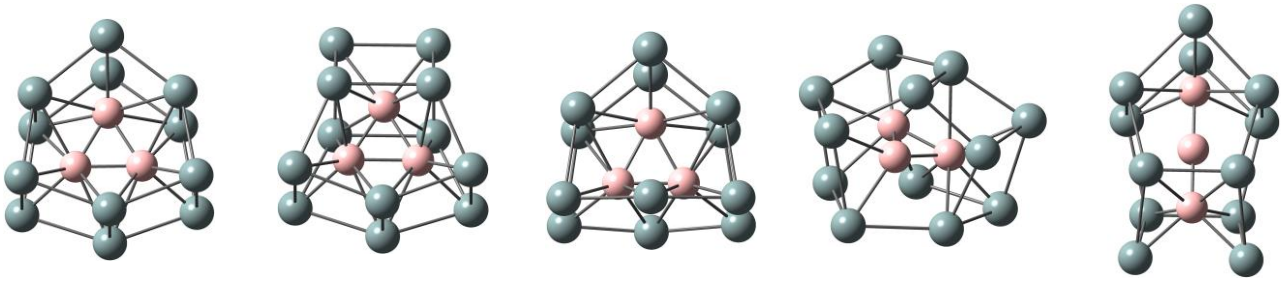
12n.1 (C_s, ^{1}A') 0.0 [0.0] (0.0) {0.0}

12n.2 (C_s, ^{1}A') 2.4 [2.1] (1.2) {2.9}

12n.3 (C_s, ^{1}A') 9.5 [10.1] (9.2) {10.1}

12n.4 (C_2, ^{1}A) 10.8 [11.3] (10.9) {11.9 }

Figure S2.



12c.1 (D_{3h}, ^{1}A'$_1$) 0.0 [0.0] (0.0) {0.0}

12c.2 (C_{2v}, ^{1}A$_1$) 21.3 [26.9] (28.0) {25.3}

12c.3 (C_{2v}, ^{1}A$_1$) - [32.6] (31.0) {30.2}

12c.4 (C_1, ^{1}A) - [35.9] (36.3) {33.7}

12c.5 (D_{2d}, ^{1}A$_1$) - [39.4] (30.1) {36.4}

Figure S3.

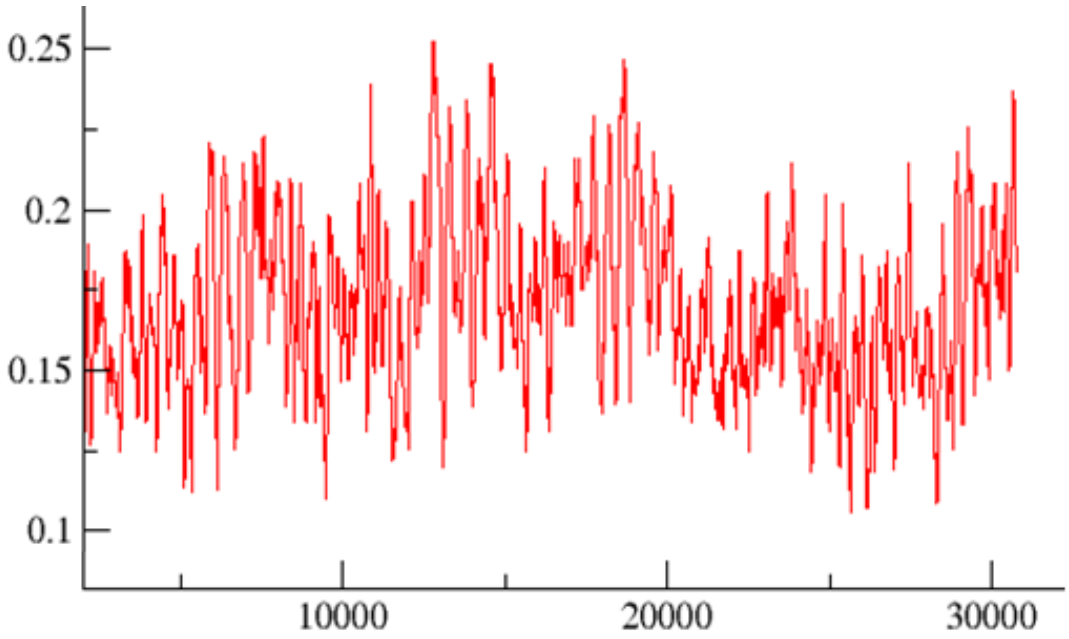
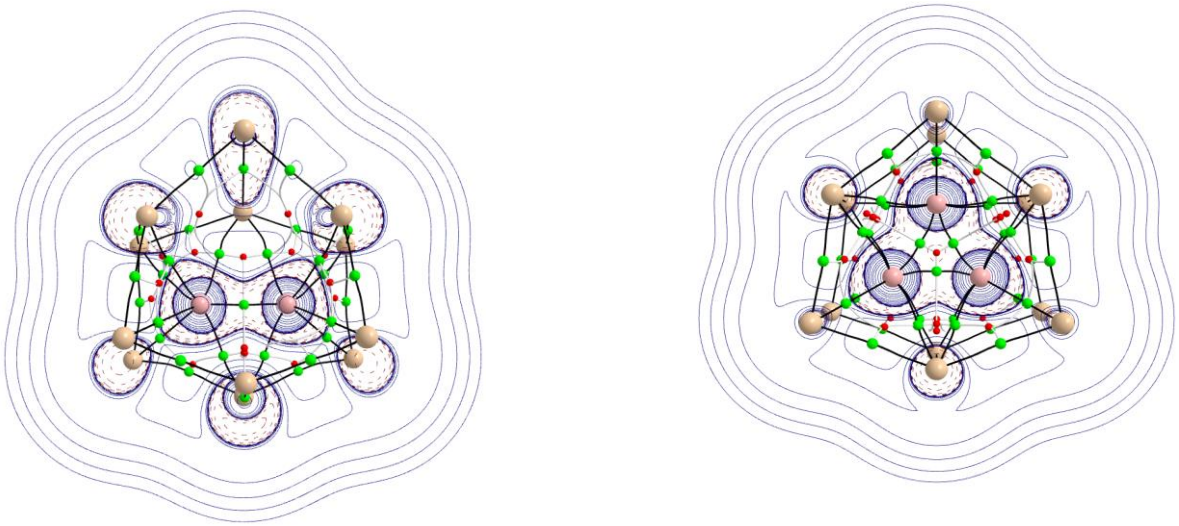
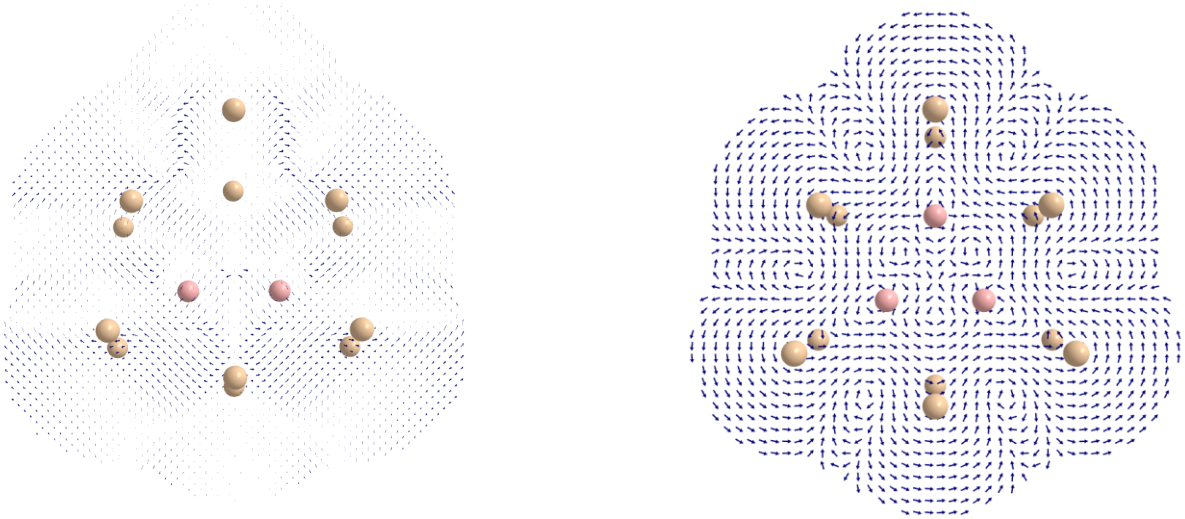


Figure S4.



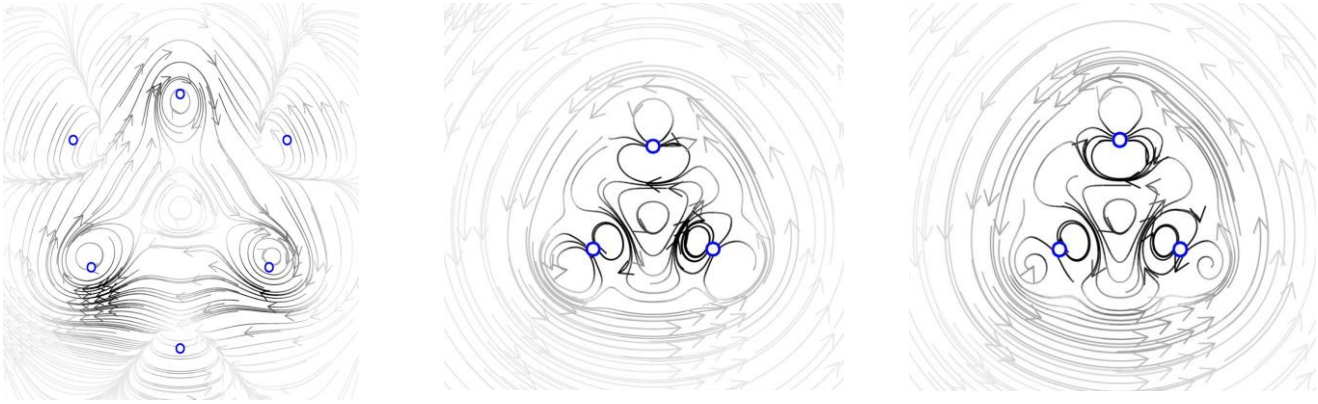
B_2Si_{12} **$B_3Si_{12}^+$**

Figure S5.



B_2Si_{12} **$B_3Si_{12}^+$**

Figure S6.



Si_{12} B_3^+ B_3^-

Figure S7.

Table: Cartesian coordinates of **3.cA**, **2.n.A** and **1.c.A**

3.c.A

B	0.00000000	-1.00494006	0.00000000
B	0.87030362	0.50247003	0.00000000
B	-0.87030362	0.50247003	0.00000000
Si	0.00000000	2.20478101	1.18333109
Si	2.29172883	1.32313025	1.30965506
Si	1.90939637	-1.10239051	1.18333109
Si	-0.00000000	-2.64626051	-1.30965506
Si	-0.00000000	-2.64626051	1.30965506
Si	-2.29172883	1.32313025	1.30965506
Si	-1.90939637	-1.10239051	-1.18333109
Si	-2.29172883	1.32313025	-1.30965506
Si	-0.00000000	2.20478101	-1.18333109
Si	1.90939637	-1.10239051	-1.18333109
Si	2.29172883	1.32313025	-1.30965506
Si	-1.90939637	-1.10239051	1.18333109

2.n.A

Si	-1.48281604	0.86365693	-2.26025190
Si	-1.13899367	1.59294541	0.00000000
Si	-1.48281604	0.86365693	2.26025190
Si	-0.98685470	-1.56123830	2.35442720
Si	-0.72896363	-2.31277486	0.00000000
Si	-0.98685470	-1.56123830	-2.35442720
Si	1.45932666	-0.86854169	2.22614710
Si	1.55383787	-1.69446015	0.00000000
Si	1.45932666	-0.86854169	-2.22614710
Si	0.82328736	1.39062725	1.85031800
Si	0.82328736	1.39062725	-1.85031800
Si	0.81228090	3.00892043	0.00000000
B	-0.17366723	-0.34109487	-0.88098190
B	-0.17366723	-0.34109487	0.88098190

1.c.A

B	-0.25473299	-0.00013102	0.00000000
Si	-2.35751886	0.46565460	0.00000000
Si	-0.72032657	1.44354011	1.67576300
Si	1.18291391	-0.32360645	-1.68554400
Si	0.36025537	-2.14335020	0.00000000
Si	-0.17844399	0.00042195	3.59052900
Si	1.18291391	-0.32360645	1.68554400
Si	-1.23308334	-1.16338073	-1.65529300

Si	2.94132901	0.00181103	0.00000000
Si	1.04479053	1.76198159	0.00000000
Si	-0.17844399	0.00042195	-3.59052900
Si	-0.72032657	1.44354011	-1.67576300
Si	-1.23308334	-1.16338073	1.65529300