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

Supporting Information

Cage-like B_{39}^+ clusters with the bonding pattern of σ + π double delocalization: new members of the borospherene family

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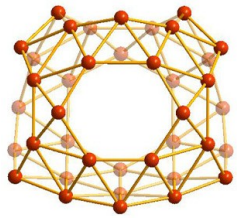
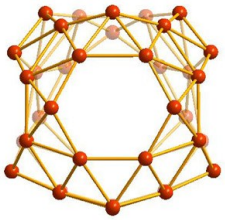
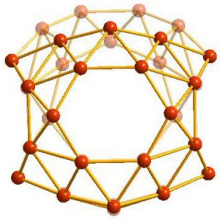
Fig. S1 Low-lying isomers of B_{39}^+ with their relative energies (with zero-point corrections included) indicated in eV at PBE0/6-311+G(d), TPSSh/6-311+G(d) (in parenthesis) and CCSD(T)/6-31G(d) (in square brackets) levels.



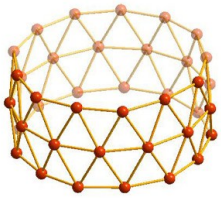
1 (C_s ^{1}A')
0.00
(0.00)
[0.00]



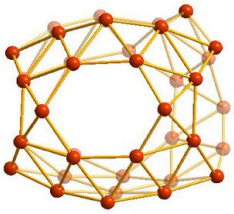
2 (C_s ^{1}A')
-0.01
(0.06)
[0.02]



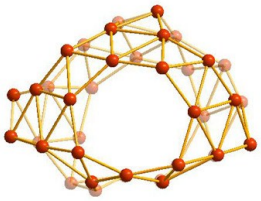
3 (C_s ^{1}A')
0.06
(0.13)
[0.13]



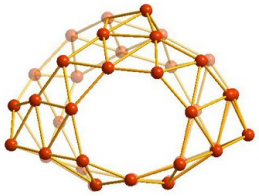
4 (C_{13} ^{1}A)
0.03
[0.24]



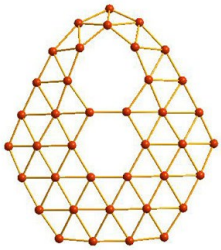
5 (C_1 ^{1}A)
0.30



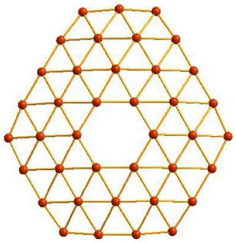
6 (C_1 ^{1}A)
0.30



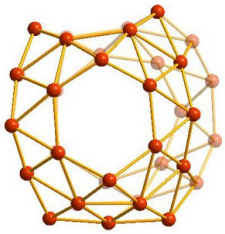
7 (C_1 ^{1}A)
0.30



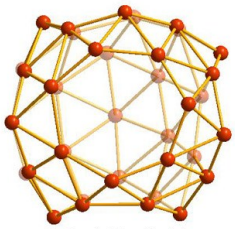
8 (C_s ^{1}A')
0.31



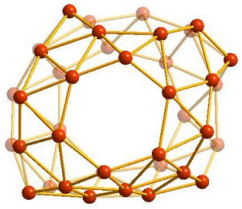
9 (C_s ^{3}A")
0.31



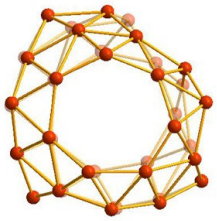
10 (C_1 ^{1}A)
0.32



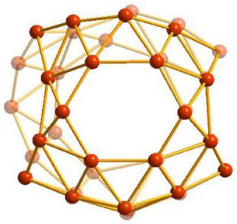
11 (C_1 ^{1}A)
0.44



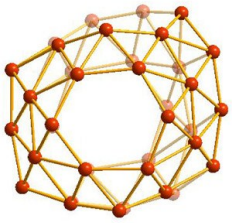
12 (C_1 ^{1}A)
0.45



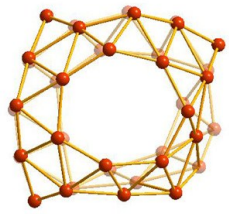
13 (C_1 ^{1}A)
0.52



14 (C_1 ^{1}A)
0.54

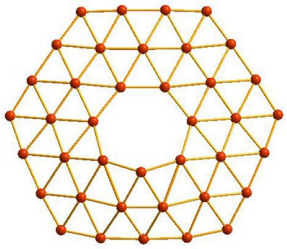


15 (C_1 ^{1}A)
0.59

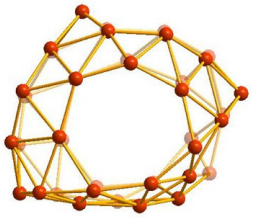


16 (C_1 ^{1}A)
0.60

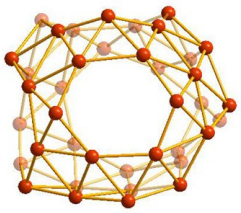
(Continued)



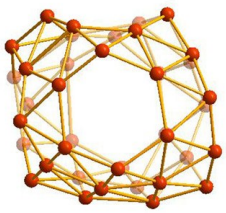
17 (C_s ^{1}A')
0.60



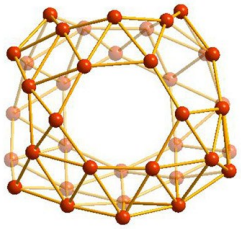
18 (C_1 ^{1}A)
0.62



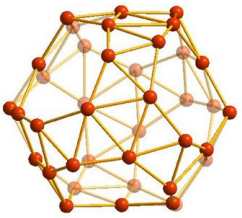
19 (C_1 ^{1}A)
0.63



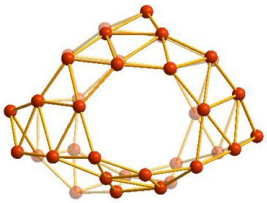
20 (C_1 ^{1}A)
0.64



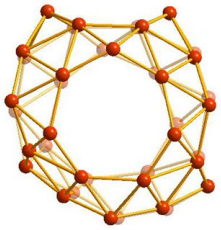
21 (C_1 ^{1}A)
0.65



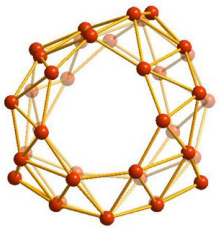
22 (C_3 ^{3}A)
0.67



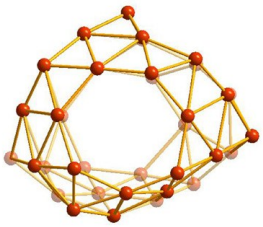
23 (C_1 ^{1}A)
0.68



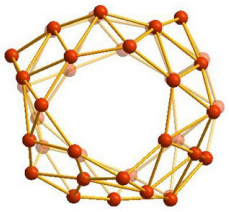
24 (C_1 ^{1}A)
0.71



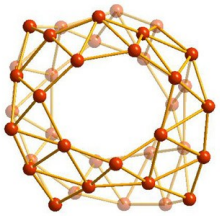
25 (C_1 ^{1}A)
0.73



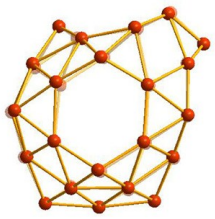
26 (C_1 ^{1}A)
0.74



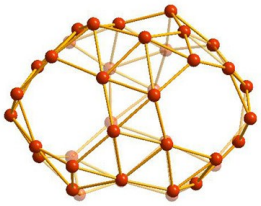
27 (C_1 ^{1}A)
0.76



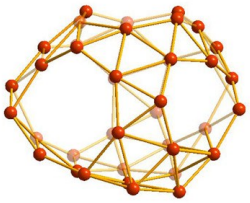
28 (C_1 ^{1}A)
0.77



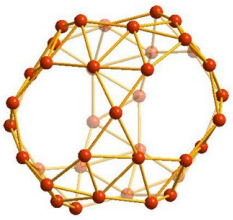
29 (C_1 ^{1}A)
0.79



30 (C_1 ^{1}A)
0.79



31 (C_1 ^{1}A)
0.82



32 (C_2 ^{1}A)
0.90

Fig.S2 Simulated IR and Raman spectrum of C_s B_{39}^+ (**3**) at PBE0/6-311+G* level.

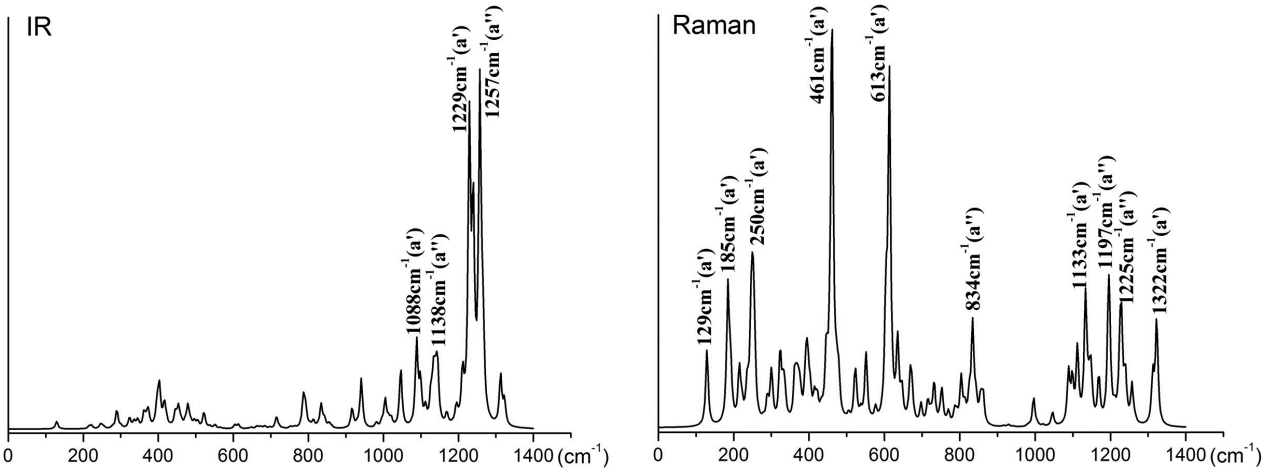


Fig.S3 Simulated UV-vis absorption spectrum of C_s B_{39}^+ (**3**) at PBE0/6-311+G* level.

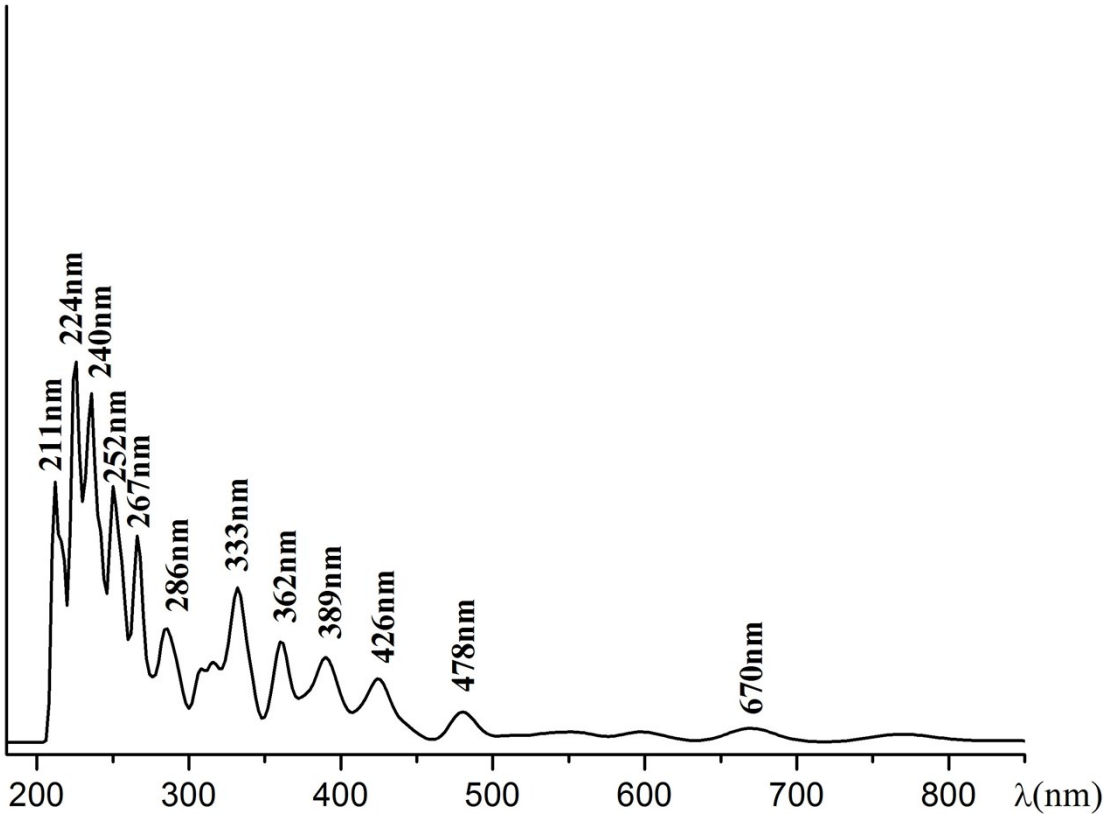


Table S1. Optimized coordinates (Å) of the first three lowest-lying isomers of B_{39}^+ at PBE0/6-311+G(d) level.

1. C_s B_{39}^+ (**1**)

B	2.96914100	−1.17000000	0.00000000
B	0.75699100	1.51935300	2.38408500
B	2.25887900	−1.36054200	1.48957700
B	−2.73925100	0.62639400	−0.84550900
B	−1.88407700	0.20841300	−2.40653400
B	2.24944600	1.55347200	−1.71012900
B	1.43611400	−1.92220500	0.00000000
B	−0.19519300	−1.66312900	2.90146100
B	0.63337500	−2.00445200	1.47657000
B	−0.03258600	3.08996100	0.00000000
B	−0.49524100	2.40677600	1.39288700
B	−2.73925100	0.62639400	0.84550900
B	−1.98205600	1.74397700	−1.72904700
B	2.25887900	−1.36054200	−1.48957700
B	−0.80372100	1.44433700	−2.74079200
B	−1.98205600	1.74397700	1.72904700
B	2.69160600	0.24728200	0.85518200
B	2.24944600	1.55347200	1.71012900
B	1.16856800	2.45844900	0.89549600
B	2.69160600	0.24728200	−0.85518200
B	1.16856800	2.45844900	−0.89549600
B	−0.80372100	1.44433700	2.74079200
B	−1.88407700	0.20841300	2.40653400
B	−0.49524100	2.40677600	−1.39288700
B	0.75699100	1.51935300	−2.38408500
B	0.63337500	−2.00445200	−1.47657000
B	−1.76535300	−1.39441200	2.79934000
B	1.83536600	0.14448000	2.39265200
B	1.83536600	0.14448000	−2.39265200
B	1.38851800	−1.36323100	2.88409400
B	−1.76535300	−1.39441200	−2.79934000
B	1.38851800	−1.36323100	−2.88409400
B	−0.19519300	−1.66312900	−2.90146100
B	−2.53994300	−1.05333600	1.42380300
B	−1.04028000	−2.01406100	1.45180100
B	−0.19641100	−2.32837600	0.00000000
B	−3.25152500	−0.66892100	0.00000000
B	−1.04028000	−2.01406100	−1.45180100
B	−2.53994300	−1.05333600	−1.42380300

C_s B_{39}^+ (**2**)

B	−2.02668600	2.02725700	−0.88267100
B	0.35812600	1.73544300	−2.31173900
B	−2.52576500	0.45327300	−1.43287300
B	1.85042000	−2.50388200	1.27918300
B	1.28441900	−1.05829300	2.08020500
B	−0.78508900	2.71020600	1.66273500
B	−2.70150800	−0.48267400	0.00000000
B	−0.56733600	−1.36816500	−2.40294300
B	−2.02288800	−1.18778200	−1.40474900
B	1.99299100	2.36883900	0.00000000
B	1.84355900	1.56255500	−1.38648200
B	2.88807500	−1.18447600	−0.89662800
B	2.61815700	0.08682500	1.81045100
B	−2.52576500	0.45327300	1.43287300
B	1.38771200	0.55029600	2.65049100
B	2.61815700	0.08682500	−1.81045100
B	−0.78508900	2.71020600	−1.66273500
B	−3.12570500	1.12605500	0.00000000
B	0.66899800	2.73246600	−0.90031600
B	−2.02668600	2.02725700	0.88267100
B	0.66899800	2.73246600	0.90031600
B	1.28441900	−1.05829300	−2.08020500
B	1.38771200	0.55029600	−2.65049100
B	1.84355900	1.56255500	1.38648200
B	0.35812600	1.73544300	2.31173900
B	−0.56733600	−1.36816500	2.40294300
B	0.44361900	−2.53178500	−1.97777300
B	−1.30671700	1.30998100	−2.32811300
B	−1.30671700	1.30998100	2.32811300
B	−1.72586600	−0.23992000	−2.72469800
B	0.44361900	−2.53178500	1.97777300
B	−1.72586600	−0.23992000	2.72469800
B	−2.02288800	−1.18778200	1.40474900
B	1.85042000	−2.50388200	−1.27918300
B	−0.78508900	−2.30378300	−0.88597200
B	−2.18473300	−2.07723700	0.00000000
B	2.82365000	−2.51543100	0.00000000
B	−0.78508900	−2.30378300	0.88597200
B	2.88807500	−1.18447600	0.89662800

3. C_s B_{39}^+ (**3**)

B	1.11331300	−2.59137800	0.90231500
B	1.69960600	−0.27251900	2.39970600
B	−0.54378700	−2.54928700	1.43948100
B	−1.10033800	2.57833000	−1.40414300
B	−0.52212000	1.33993100	−2.42809700
B	2.16512800	−1.68268200	−1.69242800
B	−1.49161400	−2.36288700	0.00000000
B	−1.49446800	−0.09207800	2.39377700
B	−1.90235700	−1.48543300	1.42983200
B	2.64904000	1.06593600	0.00000000
B	1.94425600	1.17365800	1.44040400
B	0.26929700	3.43764800	0.83585800
B	0.83310900	2.44130100	−1.96014400
B	−0.54378700	−2.54928700	−1.43948100
B	1.07063700	1.14130500	−2.85512700
B	0.83310900	2.44130100	1.96014400
B	2.16512800	−1.68268200	1.69242800
B	−0.12214400	−3.29491900	0.00000000
B	2.60046000	−0.32077600	0.87906200
B	1.11331300	−2.59137800	−0.90231500
B	2.60046000	−0.32077600	−0.87906200
B	−0.52212000	1.33993100	2.42809700
B	1.07063700	1.14130500	2.85512700
B	1.94425600	1.17365800	−1.44040400
B	0.69235500	−1.71948400	−2.37371200
B	−1.49446800	−0.09207800	−2.39377700
B	−2.04428000	1.34595300	1.83117000
B	0.69235500	−1.71948400	2.37371200
B	1.69960600	−0.27251900	−2.39970600
B	−0.91287500	−1.59134700	2.74028500
B	−2.04428000	1.34595300	−1.83117000
B	−0.91287500	−1.59134700	−2.74028500
B	−1.90235700	−1.48543300	−1.42983200
B	−1.10033800	2.57833000	1.40414300
B	−2.45147600	0.09962200	0.88805400
B	−2.76028200	−1.28665300	0.00000000
B	−1.10791800	3.37299600	0.00000000
B	−2.45147600	0.09962200	−0.88805400
B	0.26929700	3.43764800	−0.83585800