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

Electronic Supporting Information

Charge-induced structural transition between seashell-like B_{29}^- and B_{29}^+ in 18 π-electron configurations

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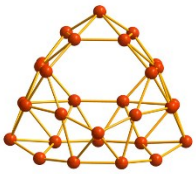
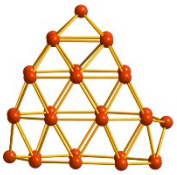
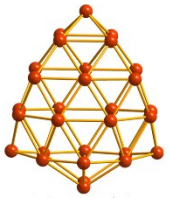
Fig.S1 Low-lying isomers of B_{29}^+ with their relative energies (with zero-point corrections included) indicated in eV at PBE0/6-311+G(d) and CCSD(T)/6-311G(d)//PBE0/6-311+G(d) (in parentheses) levels



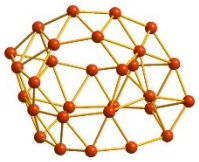
1^+ C_s ^{1}A'
0.00
(0.00)



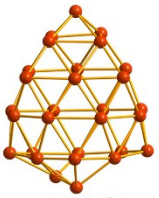
2^+ C_s ^{1}A'
+0.08
(+0.17)



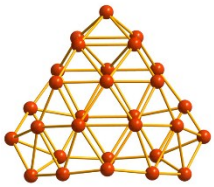
3^+ C_{2v} ^{1}A$_1$
-0.04
(+0.20)



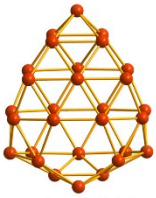
4^+ C_1 ^{1}A
+0.23
(+0.21)



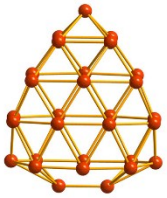
5^+ C_1 ^{1}A
-0.03
(+0.23)



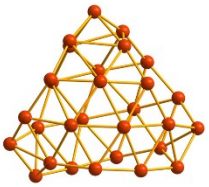
6^+ C_s ^{1}A'
+0.17
(+0.23)



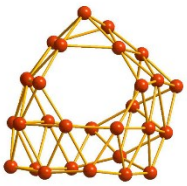
7^+ C_s ^{1}A'
-0.03
(+0.27)



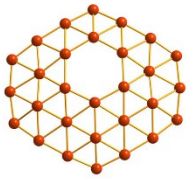
8^+ C_{2v} ^{1}A$_1$
+0.08
(+0.31)



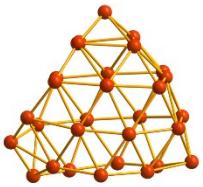
9^+ C_2 ^{1}A
+0.23
(+0.32)



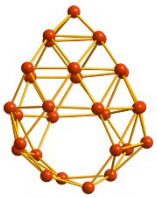
10^+ C_1 ^{1}A
+0.30
(+0.33)



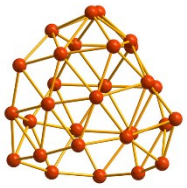
11^+ C_s ^{1}A'
+0.35
(+0.37)



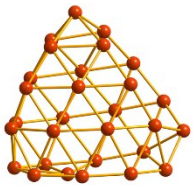
12^+ C_2 ^{1}A
+0.08
(+0.38)



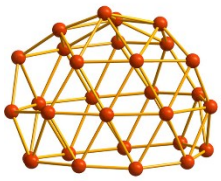
13^+ C_1 ^{1}A
+0.40
(+0.41)



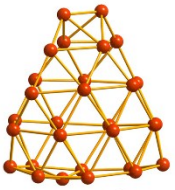
14^+ C_1 ^{1}A
+0.18
(+0.47)



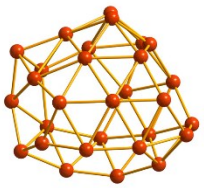
15^+ C_1 ^{1}A
+0.20
(+0.51)



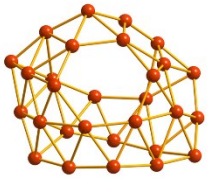
16^+ C_1 ^{1}A
+0.42
(+0.62)



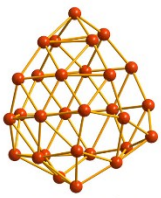
17^+ C_1 ^{1}A
+0.42
(+0.69)



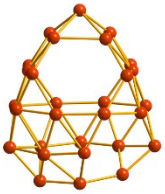
18^+ C_1 ^{1}A
+0.43



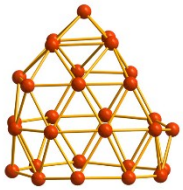
19^+ C_1 ^{1}A
+0.50



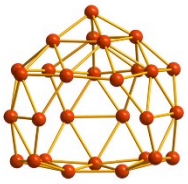
20^+ C_1 ^{1}A
+0.50



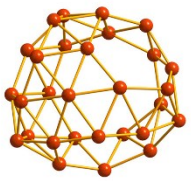
21^+ C_1 ^{1}A
+0.50



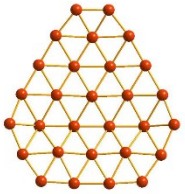
22^+ C_1 ^{1}A
+0.54



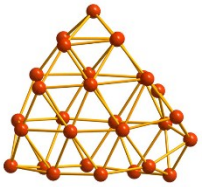
23^+ C_1 ^{1}A
+0.55



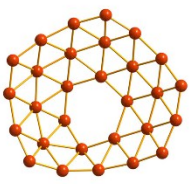
24^+ C_1 ^{1}A
+0.57



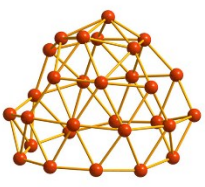
25^+ C_s ^{1}A'
+0.59



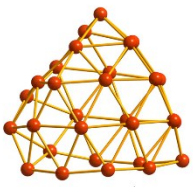
26^+ C_1 ^{1}A
+0.61



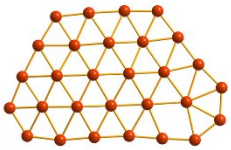
27^+ C_1 ^{1}A
+0.61



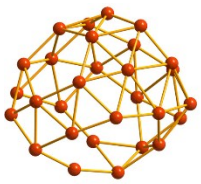
28^+ C_1 ^{1}A
+0.62



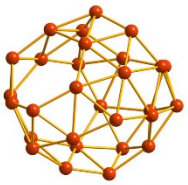
29^+ C_1 ^{1}A
+0.64



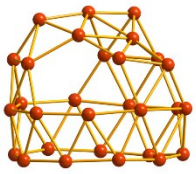
30^+ C_1 ^{1}A
+0.64



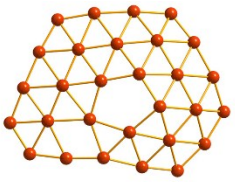
31^+ C_1 ^{1}A
+0.65



32^+ C_1 ^{1}A
+0.65



33^+ C_1 ^{1}A
+0.66



34^+ C_1 ^{1}A
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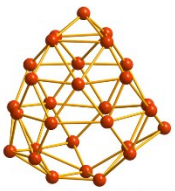
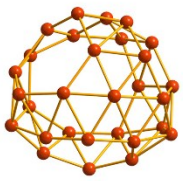
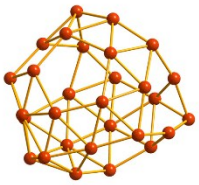


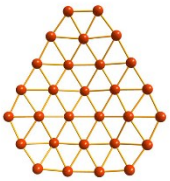
35^+ C_1 ^{1}A
+0.66



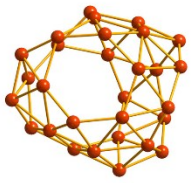
36^+ C_1 ^{1}A
+0.67



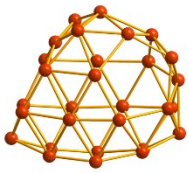
37^+ C_1 ^{1}A
+0.68



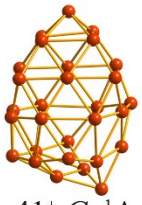
38^+ C_s ^{1}A'
+0.68



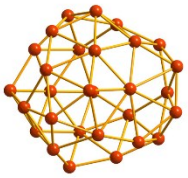
39^+ C_1 ^{1}A
+0.70



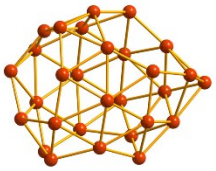
40^+ C_1 ^{1}A
+0.71



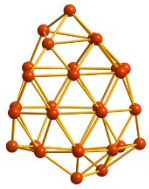
41^+ C_1 ^{1}A
+0.73



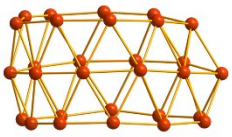
42^+ C_1 ^{1}A
+0.73



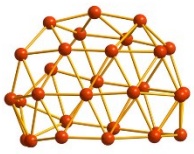
43^+ C_1 ^{1}A
+0.73



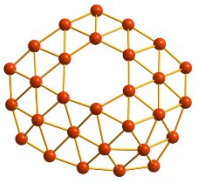
44^+ C_1 ^{1}A
+0.73



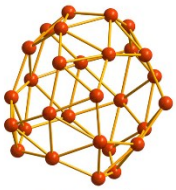
45^+ C_1 ^{1}A
+0.73
（+0.89）



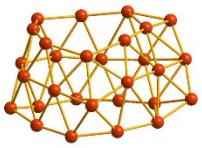
46^+ C_1 ^{1}A
+0.74



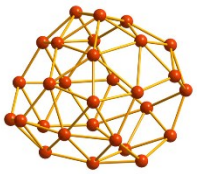
47^+ C_1 ^{1}A
+0.74



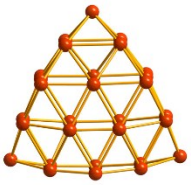
48^+ C_1 ^{1}A
+0.76



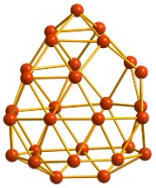
49^+ C_1 ^{1}A
+0.76



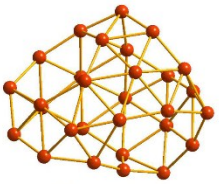
50^+ C_1 ^{1}A
+0.76



51^+ C_{2v} ^{1}A$_1$
+0.76



52^+ C_1 ^{1}A
+0.76



53^+ C_1 ^{1}A
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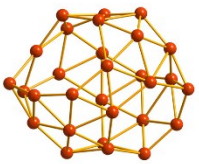
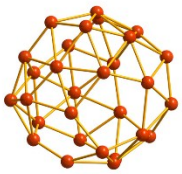


54^+ C_1 ^{1}A
+0.79



55^+ C_1 ^{1}A
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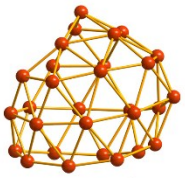
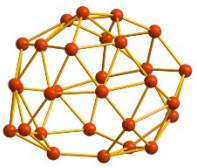
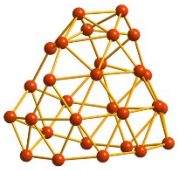


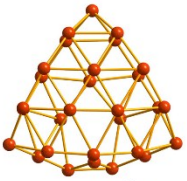
56^+ C_1 ^{1}A
+0.79



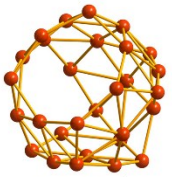
57^+ C_1 ^{1}A
+0.80



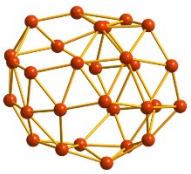
58^+ C_1 ^{1}A
+0.80



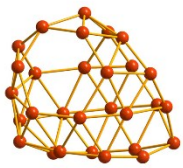
59^+ C_1 ^{1}A
+0.81



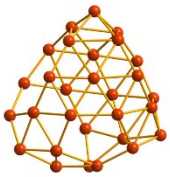
60^+ C_1 ^{1}A
+0.81



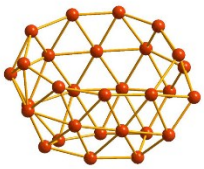
61^+ C_1 ^{1}A
+0.81



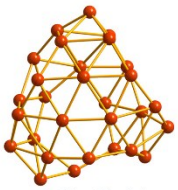
62^+ C_1 ^{1}A
+0.83



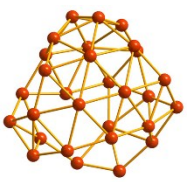
63^+ C_1 ^{1}A
+0.84



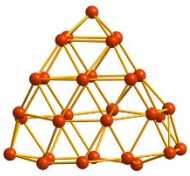
64^+ C_1 ^{1}A
+0.85



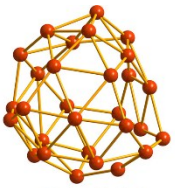
65^+ C_1 ^{1}A
+0.85



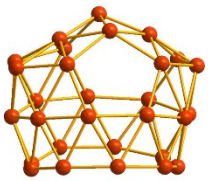
66^{+} C_1 ^{1}A
+0.86



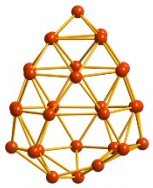
67^{+} C_1 ^{1}A
+0.86



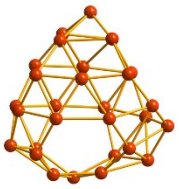
68^{+} C_1 ^{1}A
+0.87



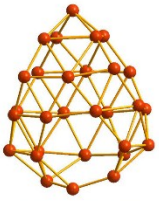
69^{+} C_1 ^{1}A
+0.88



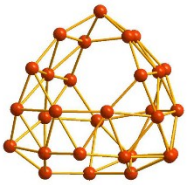
70^{+} C_1 ^{1}A
+0.88



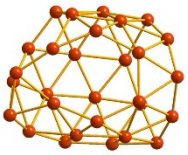
71^{+} C_1 ^{1}A
+0.88



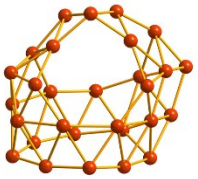
72^{+} C_1 ^{1}A
+0.88



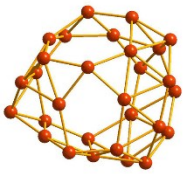
73^{+} C_1 ^{1}A
+0.89



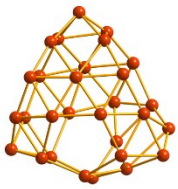
74^{+} C_1 ^{1}A
+0.89



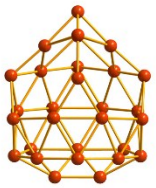
75^{+} C_1 ^{1}A
+0.89



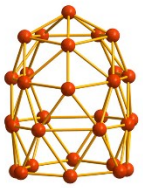
76^{+} C_1 ^{1}A
+0.89



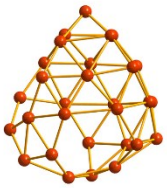
77^{+} C_1 ^{1}A
+0.89



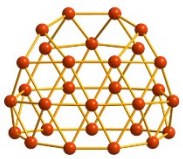
78^{+} C_s ^{1}A’
+0.90



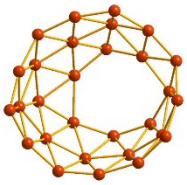
79^{+} C_s ^{1}A’
+0.90



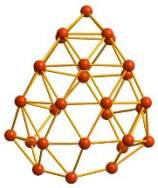
80^{+} C_1 ^{1}A
+0.90



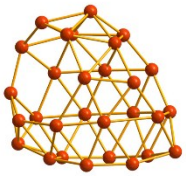
81^{+} C_s ^{1}A’
+0.90



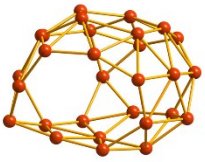
82^{+} C_1 ^{1}A
+0.90



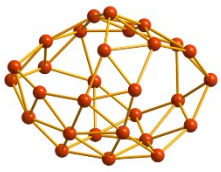
83^{+} C_1 ^{1}A
+0.91



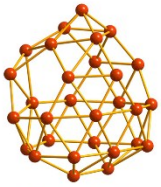
84^{+} C_1 ^{1}A
+0.91



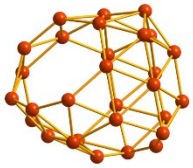
85^{+} C_1 ^{1}A
+0.91



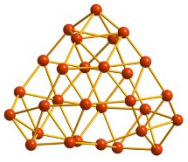
86^{+} C_1 ^{1}A
+0.91



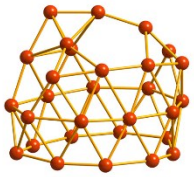
87^{+} C_1 ^{1}A
+0.91



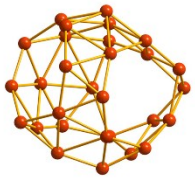
88^{+} C_1 ^{1}A
+0.92



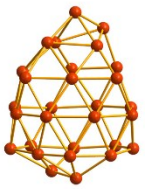
89^{+} C_1 ^{1}A
+0.92



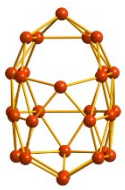
90^{+} C_1 ^{1}A
+0.92



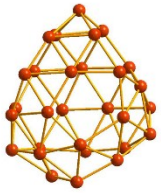
91^{+} C_1 ^{1}A
+0.92



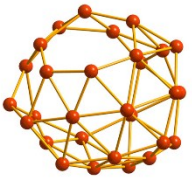
92^{+} C_1 ^{1}A
+0.93



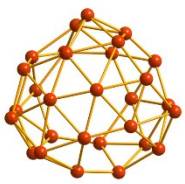
93^{+} C_s ^{1}A’
+0.93



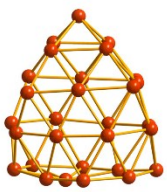
94^{+} C_1 ^{1}A
+0.93



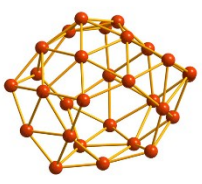
95^{+} C_1 ^{1}A
+0.94



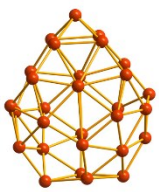
96^{+} C_1 ^{1}A
+0.94



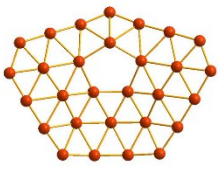
97^{+} C_1 ^{1}A
+0.94



98^{+} C_1 ^{1}A
+0.95



99^{+} C_2 ^{1}A
+0.96



100^{+} C_s ^{1}A’
+1.62

Fig.S2 Born-Oppenheimer molecular dynamics simulations of C_s B_{29}^+ (**1**$^+$) at 500K, 700K and 1000K for 30 ps. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

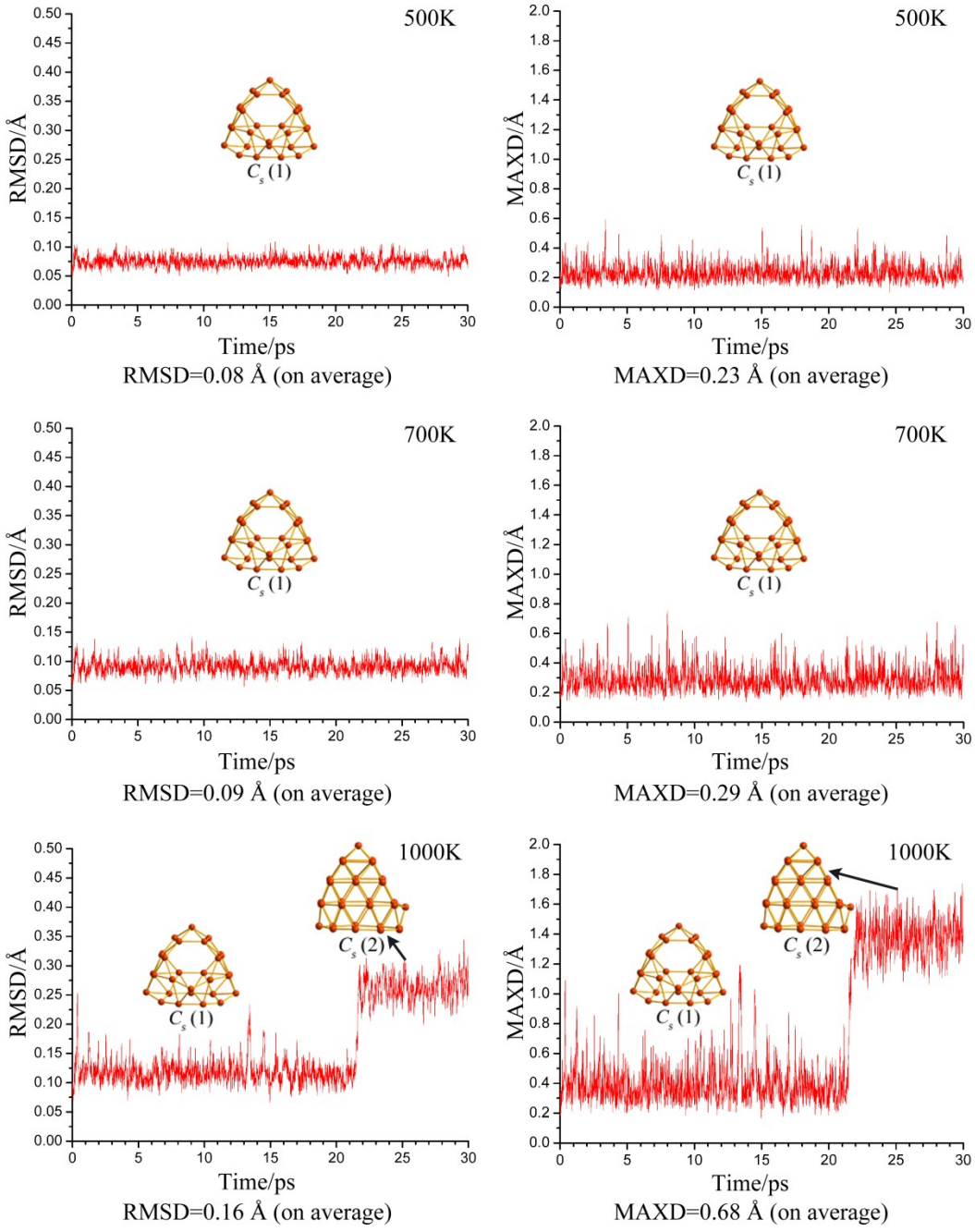


Table S1 optimized coordinates (Å) of the five lowest-lying isomers of B_{29}^+ at PBE0/6-311+G(d)

1. C_s B_{29}^+ (**1**$^+$)

B	2.57394800	0.11795900	1.16305200
B	-0.50464600	0.51087100	-2.55568600
B	-2.12182700	-0.40408100	-2.03616500
B	-1.29637700	1.46584000	-1.30088400
B	-0.89589400	-1.55360300	1.50798300
B	0.22199000	1.74581800	-1.84233700
B	1.08660500	0.38841900	-2.04522800
B	1.93557800	-1.07049200	-1.98835600
B	-0.62643400	-1.95789800	0.00000000
B	1.08660500	0.38841900	2.04522800
B	-1.10276400	-0.97690300	-3.07784000
B	-2.12182700	-0.40408100	2.03616500
B	-1.29637700	1.46584000	1.30088400
B	0.76159200	-1.63033900	-0.85391900
B	0.44167300	-1.19649200	2.61788700
B	-1.10276400	-0.97690300	3.07784000
B	0.76159200	-1.63033900	0.85391900
B	-0.50464600	0.51087100	2.55568600
B	2.87334700	1.18161700	0.00000000
B	-0.89589400	-1.55360300	-1.50798300
B	0.22199000	1.74581800	1.84233700
B	1.93557800	-1.07049200	1.98835600
B	1.56609600	1.60801500	-0.87405000
B	1.56609600	1.60801500	0.87405000
B	0.44167300	-1.19649200	-2.61788700
B	-2.70294300	0.49664200	-0.83939400
B	2.57394800	0.11795900	-1.16305200
B	-2.70294300	0.49664200	0.83939400
B	-2.17297400	1.77297300	0.00000000

2. C_s B_{29}^+ (**2**$^+$)

B	0.14886000	0.65823400	2.21435100
B	-2.45332100	-0.15150600	1.35563400
B	2.48160800	-2.17090300	0.00000000
B	-0.62633000	2.15998100	1.90139500
B	-0.62633000	2.15998100	-1.90139500
B	-1.56820600	0.90388200	2.18705600
B	-2.45332100	-0.15150600	-1.35563400
B	2.28384000	-0.87804500	-0.93020500
B	0.09664500	3.07891300	0.82660500
B	-0.31685700	-2.13644500	-1.56395600

B	-0.31685700	-2.13644500	1.56395600
B	-1.76042200	-1.66820900	-0.85686500
B	0.14886000	0.65823400	-2.21435100
B	1.75128000	0.36583000	1.77207300
B	0.70838900	-0.92498700	-1.95486600
B	1.09551900	1.85535900	-1.47007300
B	1.38530600	2.51783300	0.00000000
B	0.09664500	3.07891300	-0.82660500
B	-1.56820600	0.90388200	-2.18705600
B	1.13850300	-2.30793000	-0.88303300
B	1.75128000	0.36583000	-1.77207300
B	2.28384000	-0.87804500	0.93020500
B	0.70838900	-0.92498700	1.95486600
B	-2.93537900	-0.87886800	0.00000000
B	1.09551900	1.85535900	1.47007300
B	-1.76042200	-1.66820900	0.85686500
B	1.13850300	-2.30793000	0.88303300
B	-0.96366700	-0.68910900	-2.03355300
B	-0.96366700	-0.68910900	2.03355300

3. C_{2v} B_{29}^{+} (**3**$^{+}$)

B	-0.90396300	2.04428600	-0.23154700
B	-0.87629600	0.99290400	2.39803500
B	2.25091200	0.92248800	-0.17142500
B	-2.25091200	0.92248800	-0.17142500
B	-0.90396300	-2.04428600	-0.23154700
B	-1.71956100	1.65916800	1.17409800
B	0.00000000	0.00000000	3.32235400
B	1.40986100	-1.21160800	-1.67504400
B	-1.40986100	1.21160800	-1.67504400
B	2.25091200	-0.92248800	-0.17142500
B	0.00000000	1.80874800	1.15857500
B	1.71956100	-1.65916800	1.17409800
B	0.00000000	-1.80874800	1.15857500
B	0.00000000	2.09184400	-1.68161200
B	0.90396300	-2.04428600	-0.23154700
B	-1.40986100	-1.21160800	-1.67504400
B	-2.25091200	-0.92248800	-0.17142500
B	-2.49612800	0.00000000	-1.49628500
B	-1.71956100	-1.65916800	1.17409800
B	2.49612800	0.00000000	-1.49628500
B	0.00000000	-0.81641600	-2.63009100
B	1.40986100	1.21160800	-1.67504400
B	0.90396300	2.04428600	-0.23154700

B	-0.87629600	-0.99290400	2.39803500
B	0.00000000	-2.09184400	-1.68161200
B	0.87629600	0.99290400	2.39803500
B	0.00000000	0.81641600	-2.63009100
B	0.87629600	-0.99290400	2.39803500
B	1.71956100	1.65916800	1.17409800

4. C_1 B_{29}^+ (**4**$^+$)

B	-0.79519000	2.57702300	0.45374100
B	2.22421800	0.45947000	-0.79054700
B	1.74056800	-2.53785700	0.09672300
B	0.41595800	-2.58385800	-0.75689400
B	-1.79342100	-1.14277300	1.38373200
B	1.16319000	0.01661300	-1.94524500
B	3.01166000	1.43120800	0.49720900
B	2.14510900	0.14537000	1.33594800
B	-0.30498800	-1.22285400	1.90834000
B	-1.98523000	1.40986800	-0.09829300
B	2.79321300	-1.39747700	0.45383600
B	-2.33767200	-1.75340600	-0.31912200
B	-1.53211900	-0.69341400	-1.59865500
B	0.70791900	0.01590800	2.03015300
B	-2.54887800	0.43160400	1.27232900
B	-3.26796000	-0.95844700	0.66699200
B	-0.88636700	0.39134400	1.80883400
B	-2.80881400	0.02838000	-0.59784900
B	0.43390000	2.86446500	-0.58491300
B	1.22157600	-1.40841900	1.25912200
B	-1.98706100	0.90366600	-1.64474800
B	-1.71215800	1.83138300	1.51196800
B	0.92158900	1.53188300	-1.41001600
B	-0.74901800	1.94090800	-1.22719300
B	3.57285800	0.01180600	0.36452500
B	0.03635100	-1.18342800	-1.78462600
B	1.83654500	2.31473500	-0.12028000
B	-1.08966300	-2.24095800	-1.23431000
B	1.57388300	-1.18274300	-0.93076100

5. C_1 B_{29}^+ (**5**$^+$)

B	-0.37138600	1.89579600	-1.23390500
B	2.32116100	1.21416200	-0.62229200
B	0.84726800	-0.60769400	-2.39791500
B	-0.12766600	2.41263700	0.43740800
B	0.06166600	-0.24937500	2.12506000

B	1.13182400	2.31172300	-0.65971500
B	3.33978100	-0.05066000	-0.42520600
B	-1.66302800	-2.11647600	0.73797300
B	-1.86097000	1.20892600	-1.63615500
B	-0.27544700	-2.43684300	-0.31337400
B	0.94114500	0.89718900	-1.58237000
B	1.17077800	-2.30124300	0.34419900
B	1.39637900	-1.00373400	1.45324700
B	-1.68104100	1.82588000	-0.04804900
B	-0.10456700	-1.76638300	1.31198500
B	-1.53785800	-0.92679400	1.82932000
B	0.14979900	1.44639800	1.96157500
B	-1.29707800	2.14275900	1.51324500
B	1.52945400	0.60628200	2.06508500
B	-1.76213400	-1.99248200	-0.91173500
B	-2.44207300	-0.75551600	0.25335500
B	-0.48147000	-1.39244100	-1.77026400
B	-0.49713700	0.29555700	-2.15793900
B	2.67576300	0.13793900	1.01627000
B	-1.36243000	0.66180500	2.15076100
B	2.19647600	-0.32785900	-1.54072100
B	-2.80211100	0.61954300	-0.48314400
B	2.41419700	-1.28334100	0.06154000
B	-1.90929700	-0.46575600	-1.47824100