

Supporting Information

Sea-shell-like B_{31}^+ and B_{32} : two new axially chiral members of the borospherene family

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Fig.S1 Low-lying isomers of B_{31}^+ (a) and B_{32} (b), along with their relative energies indicated in eV at PBE0/6-311+G(d), TPSSh/6-311+G(d) (in parentheses), and CCSD(T)/6-311G(d)//PBE0/6-311+G(d) (in square brackets) levels. The energies are corrected for zero-point energies.

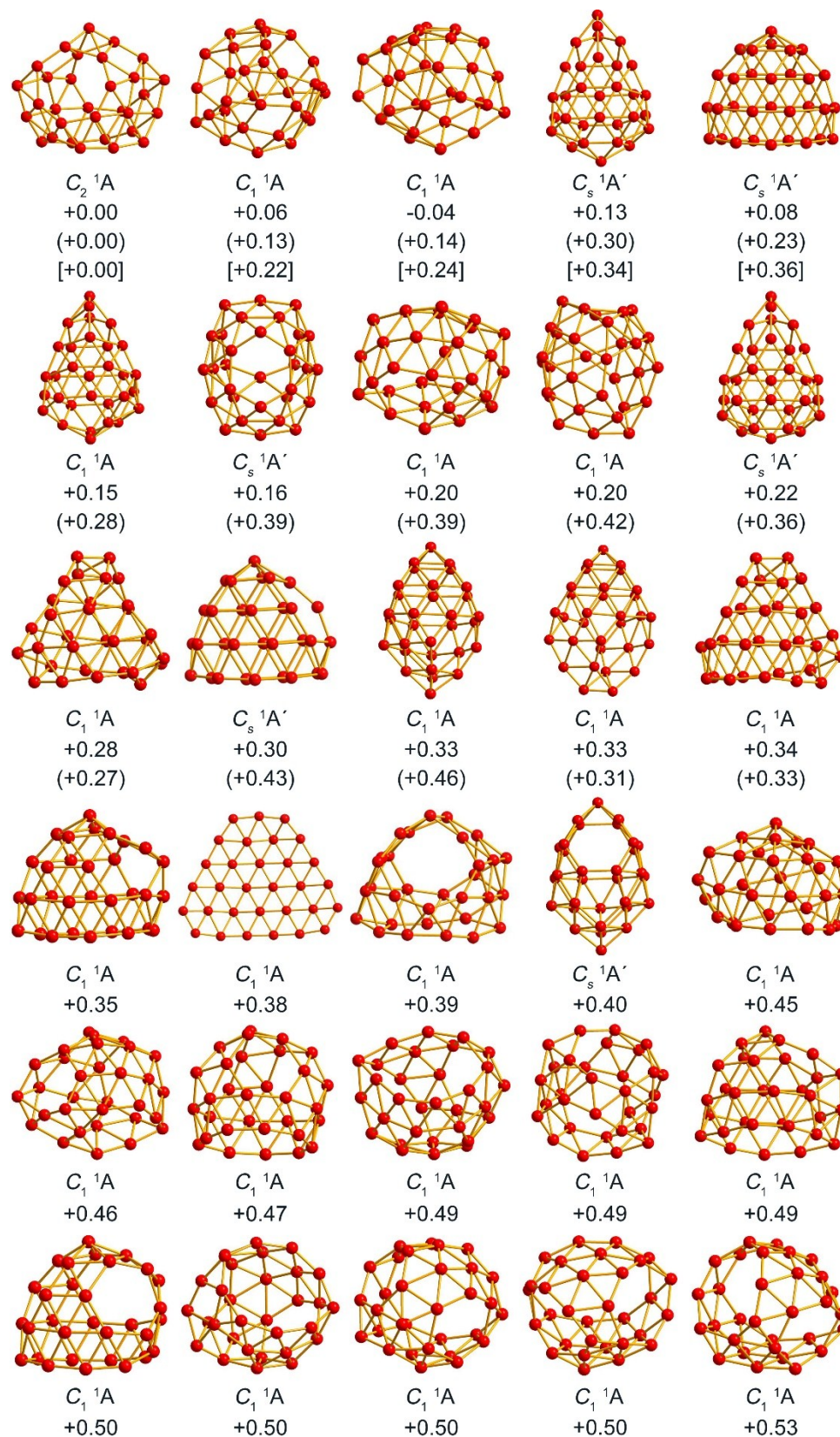
Fig.S2 Born-Oppenheimer molecular dynamics simulations of $C_2 B_{31}^+$ (c) and $C_2 B_{32}$ (d) at 500K, 700K and 1000K for 30 ps. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

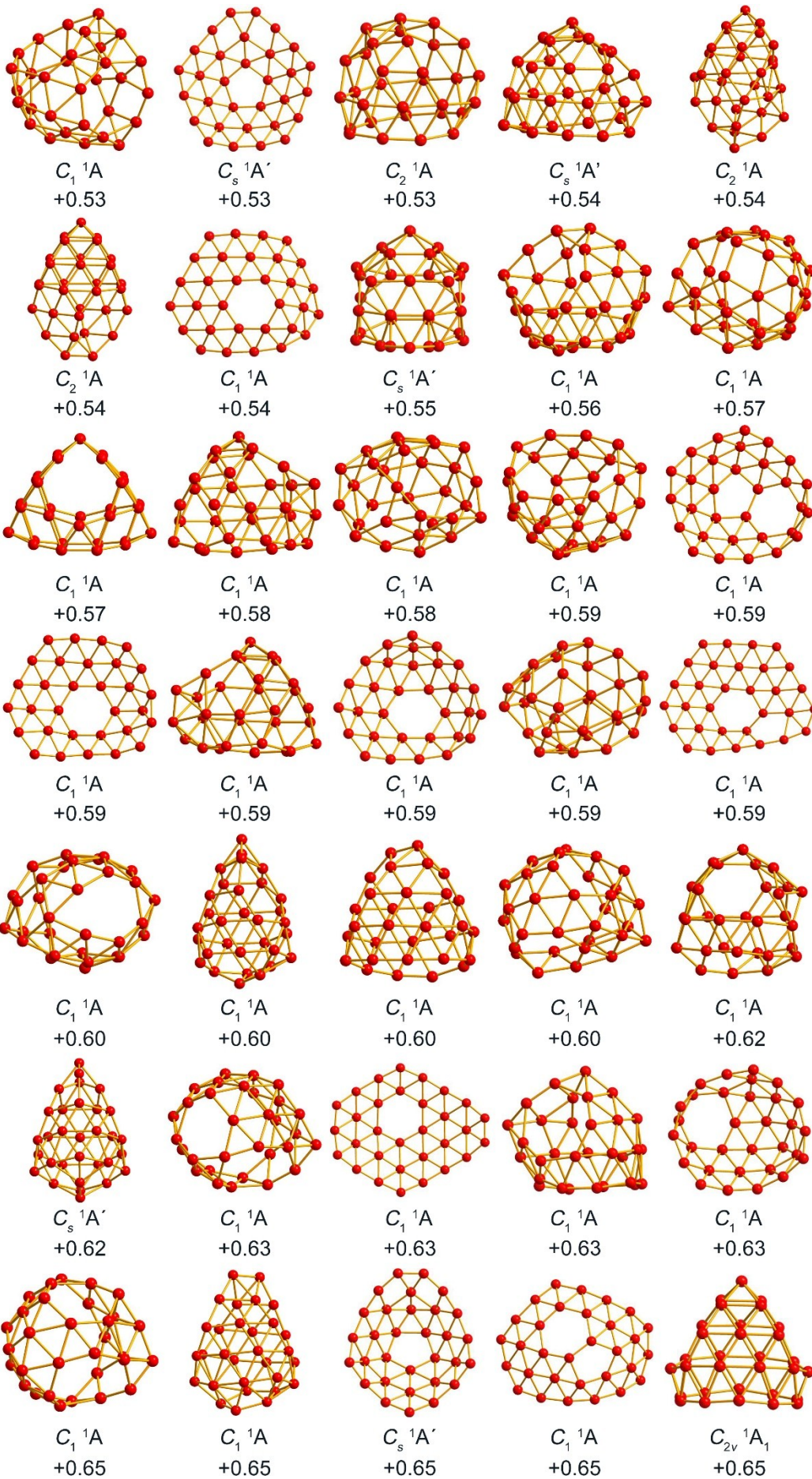
Fig. S3 σ and π AdNDP bonding patterns of $C_s B_{32}$ (VII), with the occupation numbers (ONs) indicated.

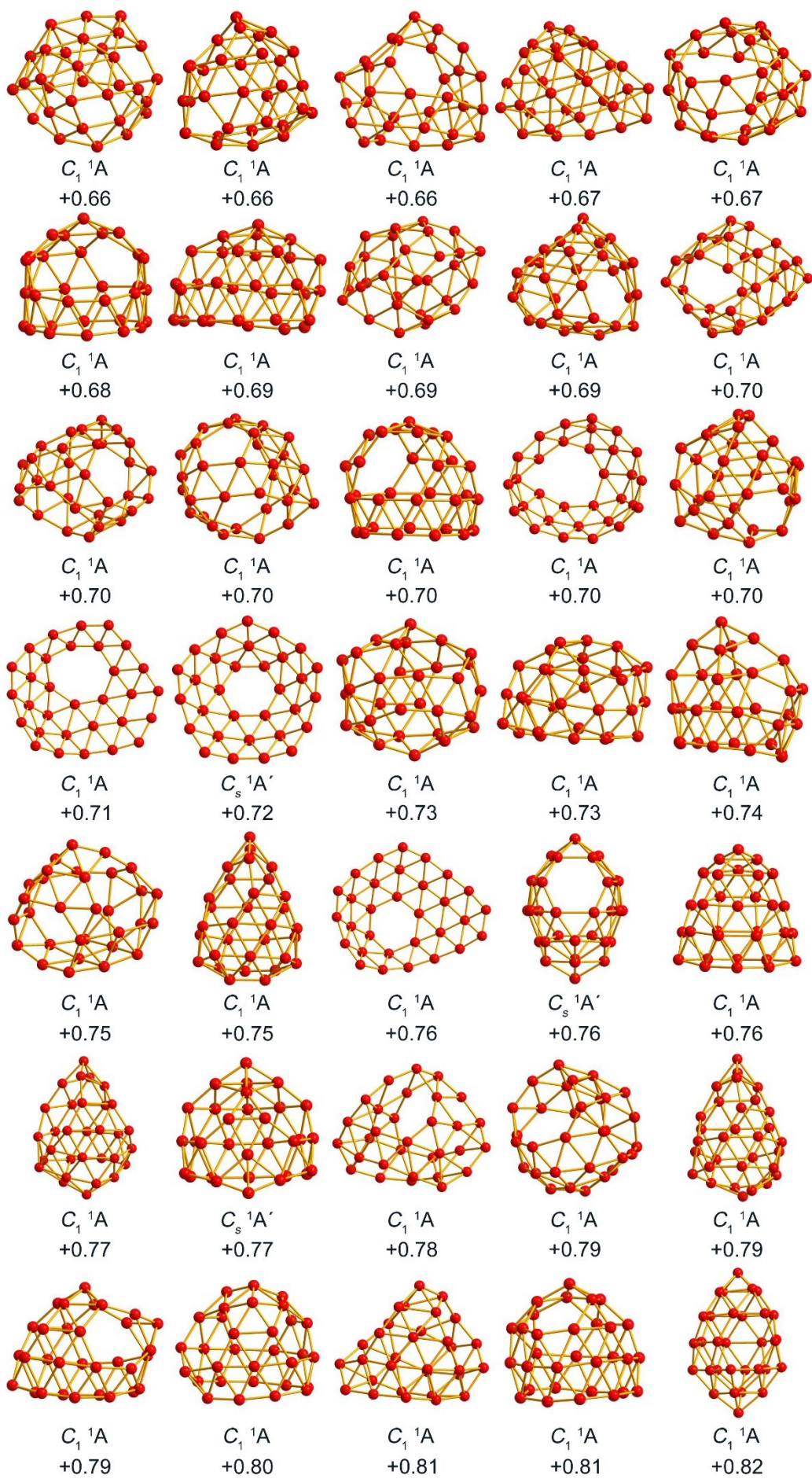
Table S1 Optimized cartesian coordinates of the GM structures of B_{31}^+ and B_{32} at PBE0/6-311+G(d)

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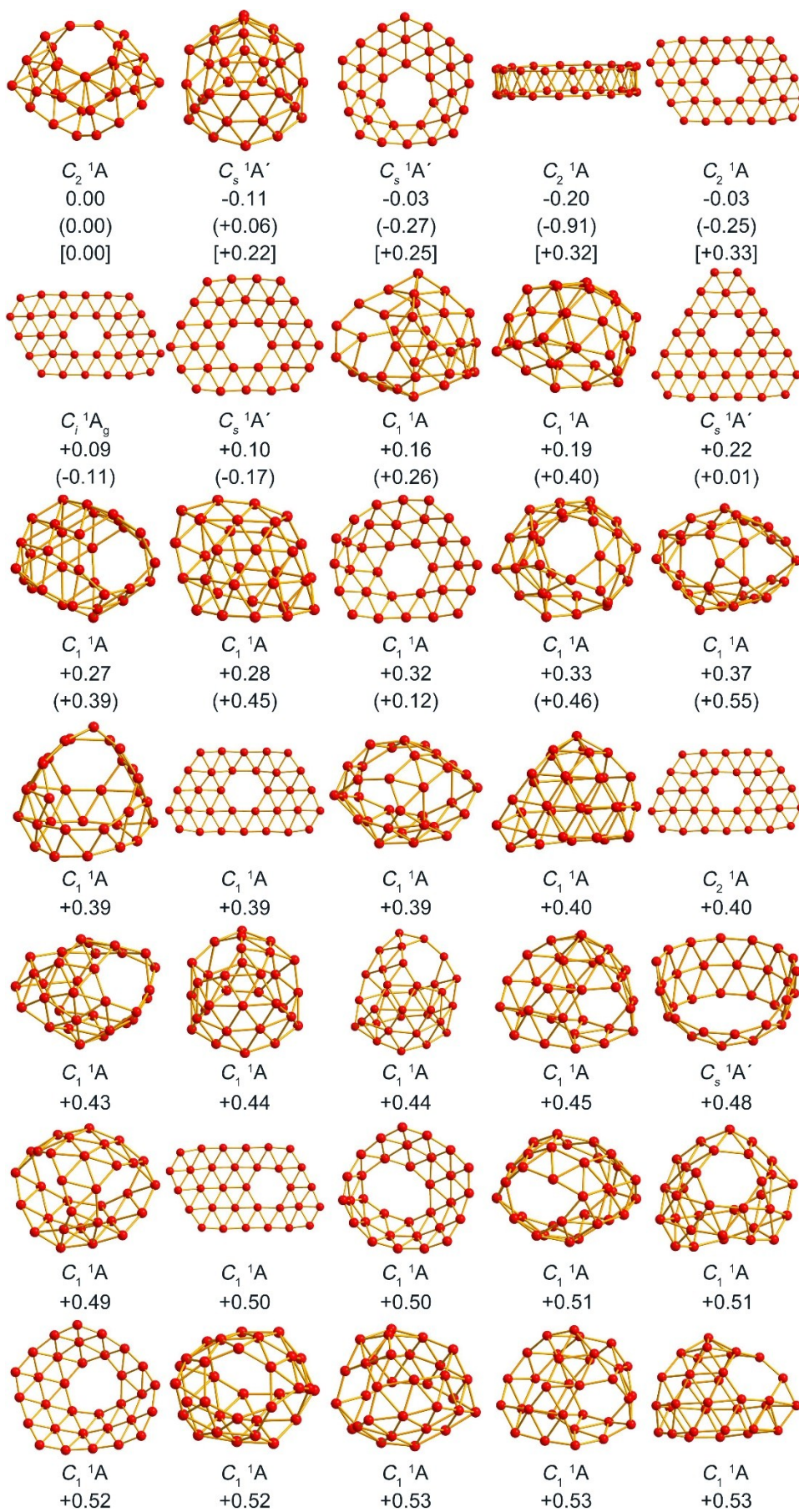
(a) B_{31}^+







(b) B₃₂



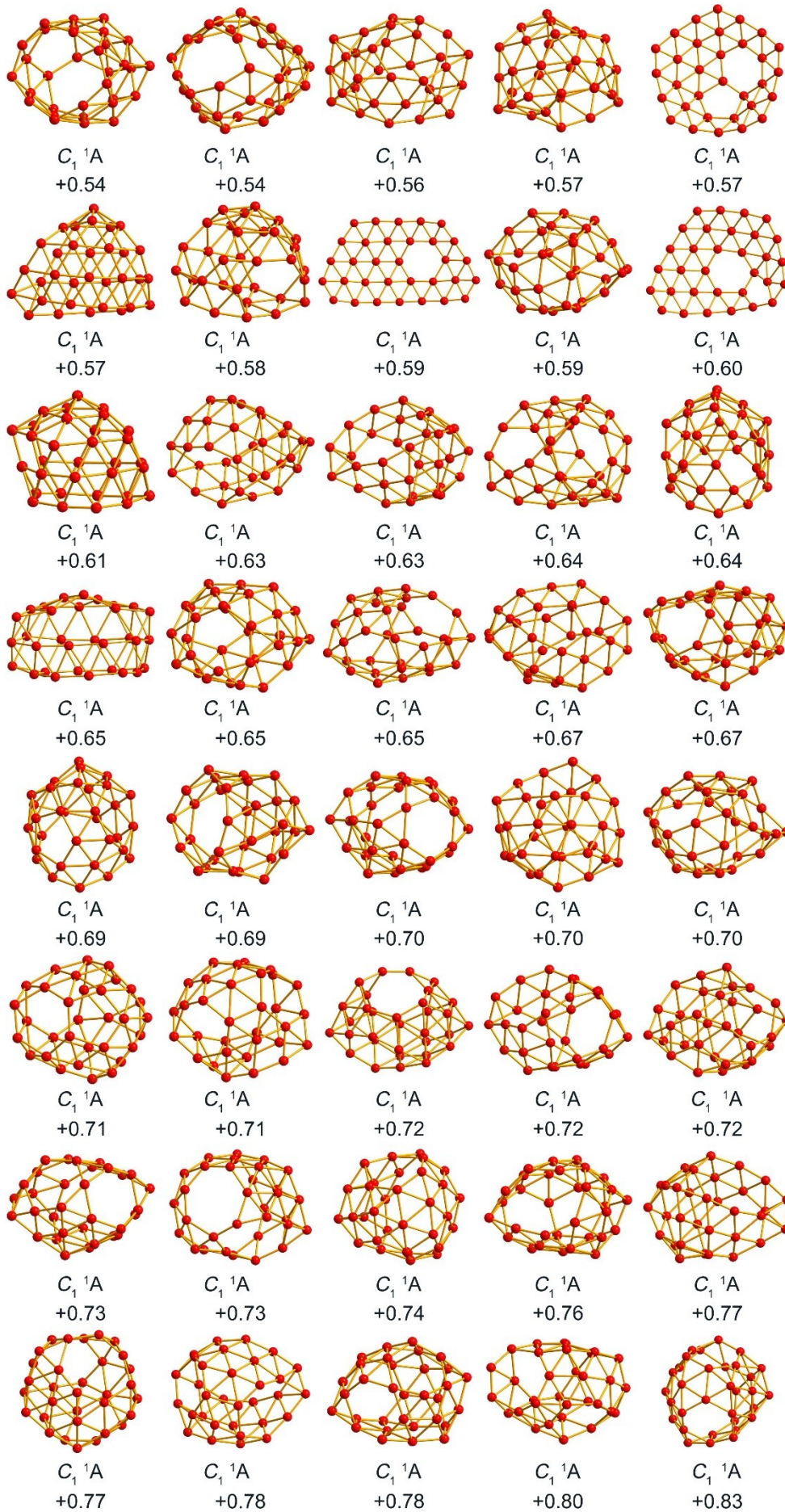
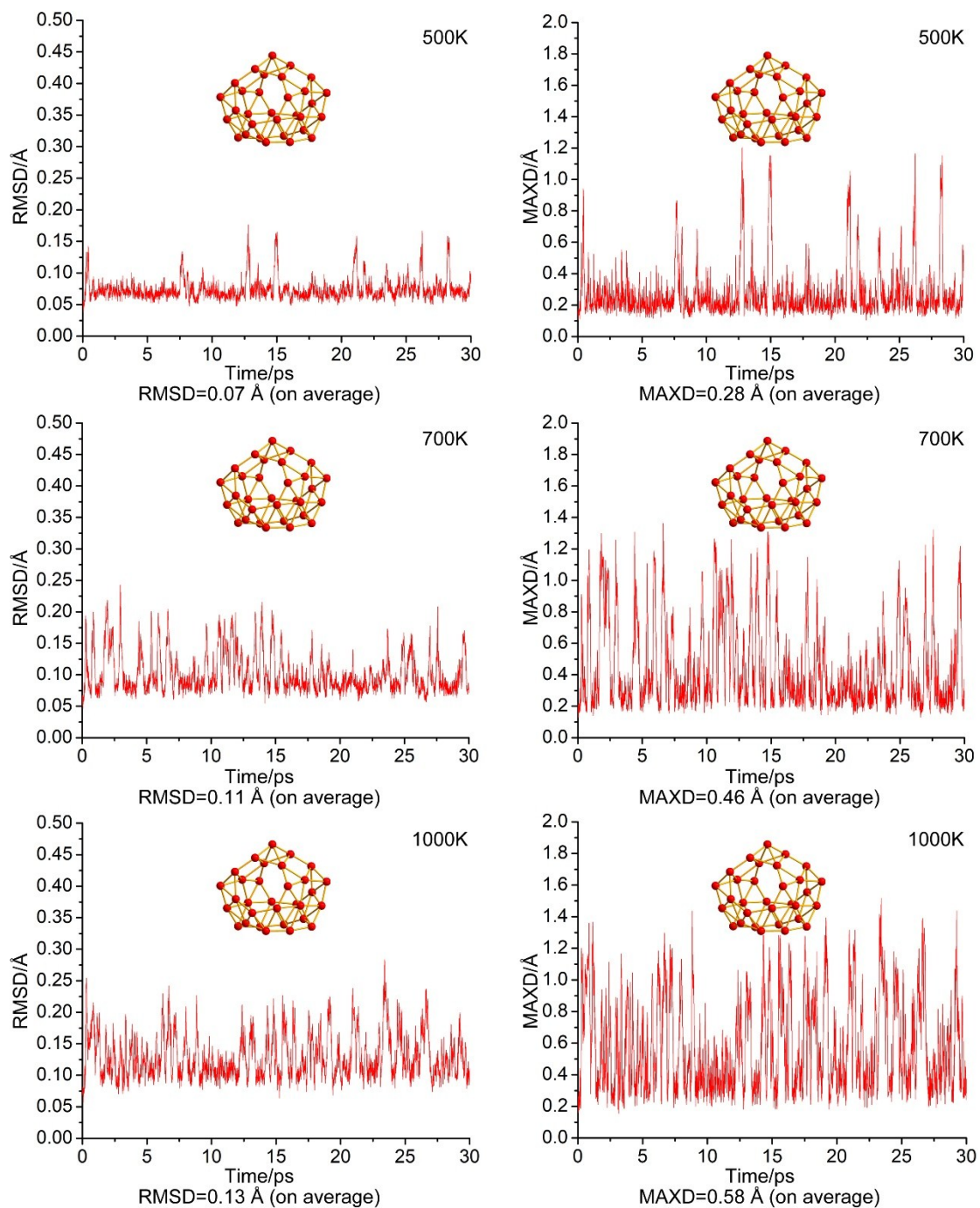


Fig.S2 Born-Oppenheimer molecular dynamics simulations of $C_2 B_{31}^+$ (a) and $C_2 B_{32}$ (b) at 500K, 700K and 1000K for 30 ps. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

(a) $C_2 B_{31}^+$



(b) $C_2 B_{32}$

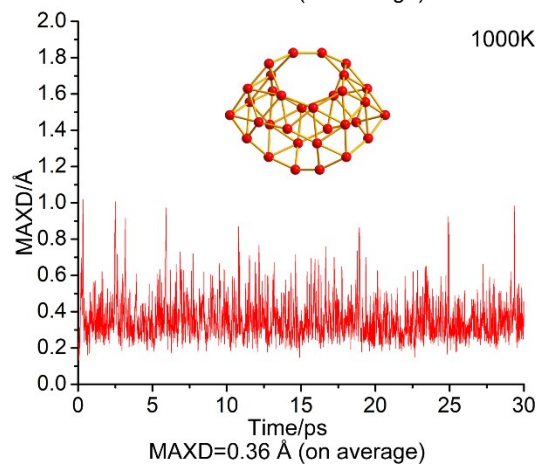
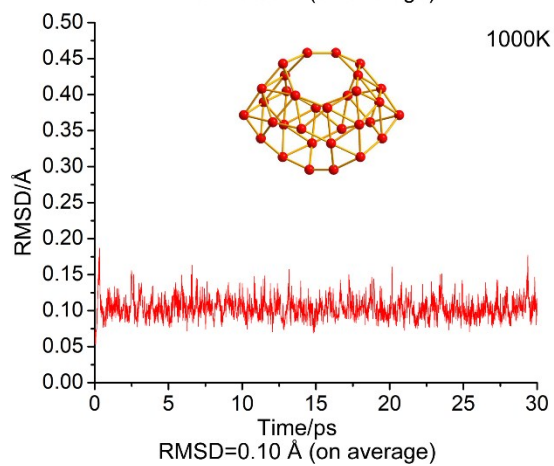
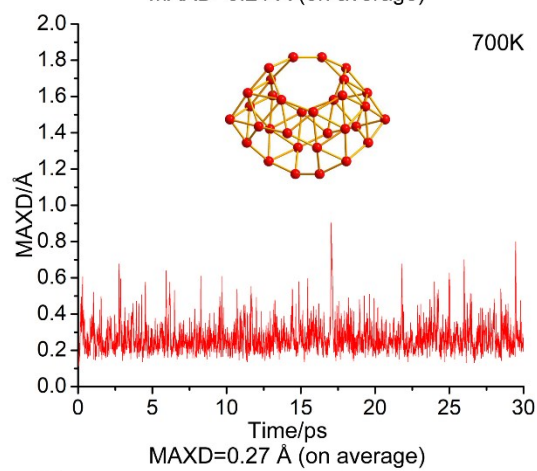
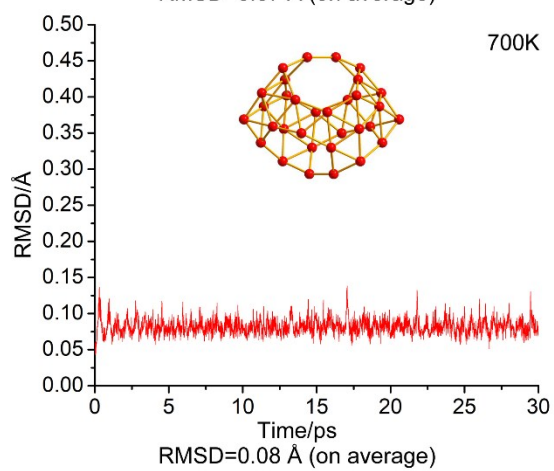
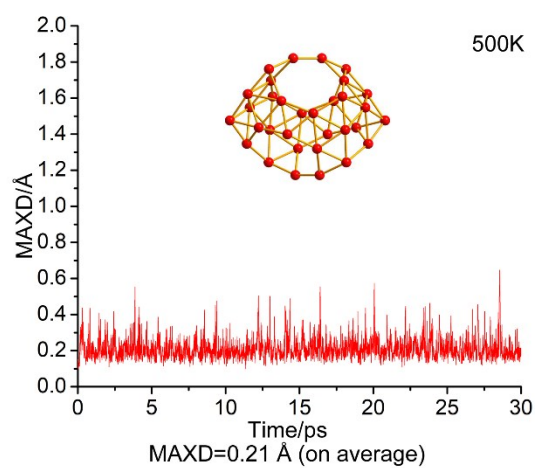
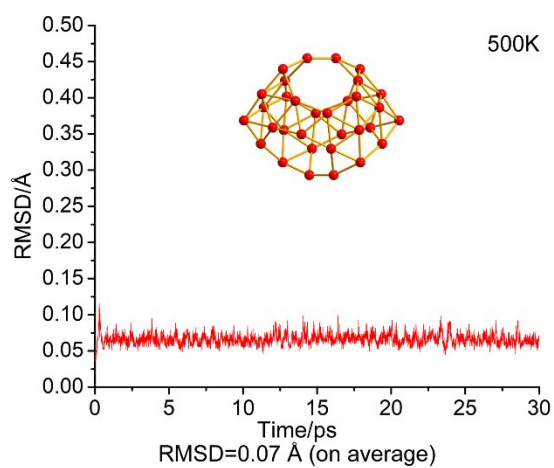


Fig. S3 σ and π AdNDP bonding patterns of C_s B_{32} (VII), with the occupation numbers (ONs) indicated.

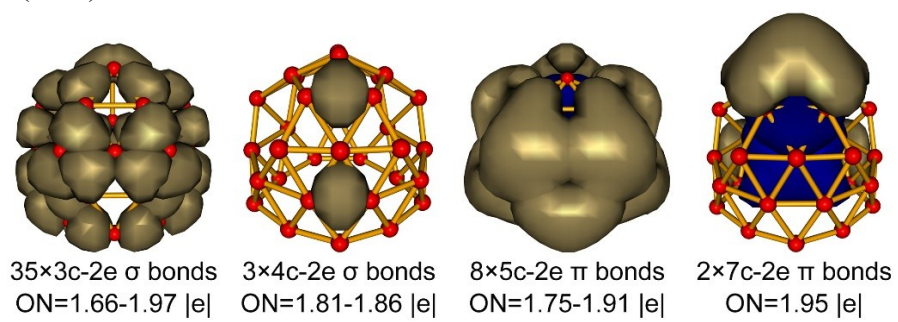


Table S1 Optimized cartesian coordinates of the GM structures of B_{31}^+ and B_{32} at PBE0/6-311+G(d)

1. $C_2 B_{31}^+$

B	-1.88265100	0.84149000	-0.61297700
B	-1.23583500	2.34274400	-0.84656300
B	1.04759800	0.08582100	2.05691600
B	-1.25600900	1.36700600	-2.10904800
B	1.85263300	1.72351000	-2.02279500
B	1.23583500	-2.34274400	-0.84656300
B	-0.23383800	-2.03425600	-1.66756000
B	1.25600900	-1.36700600	-2.10904800
B	1.72009700	0.16416000	-2.18178100
B	1.61518400	2.63926400	-0.73907300
B	0.35920600	2.65837700	1.75516700
B	0.00000000	2.85425400	0.00141400
B	1.58053200	1.47097100	1.04460400
B	1.99250200	0.85882700	-0.55731700
B	1.44478100	3.17331100	0.78737700
B	-2.04785500	0.06398100	0.79355600
B	1.88265100	-0.84149000	-0.61297700
B	0.00000000	-2.85425400	0.00141400
B	-1.85263300	-1.72351000	-2.02279500
B	0.23383800	2.03425600	-1.66756000
B	-1.72009700	-0.16416000	-2.18178100
B	-0.35920600	-2.65837700	1.75516700
B	-0.08757500	1.37087400	2.61018900
B	-1.61518400	-2.63926400	-0.73907300
B	-1.99250200	-0.85882700	-0.55731700
B	-1.58053200	-1.47097100	1.04460400
B	-1.44478100	-3.17331100	0.78737700
B	-1.04759800	-0.08582100	2.05691600
B	0.08757500	-1.37087400	2.61018900
B	2.04785500	-0.06398100	0.79355600
B	0.00000000	0.00000000	3.37578000

2. $C_2 B_{32}$

B	-1.21140200	1.89639800	2.32158200
B	-1.81198000	-1.70956800	0.97782200
B	1.24310500	-2.39542800	-0.54834700
B	-0.38349800	0.70519800	2.85201600
B	1.95187100	0.27981900	0.15532200
B	-1.60991000	-0.46586200	-1.58631900
B	-0.52354600	-0.59548300	-2.87848700
B	-0.91400200	2.93418600	1.09567500

B	-0.40123100	3.81366900	-0.19811100
B	0.79495600	2.83856900	0.43663700
B	0.40123100	-3.81366900	-0.19811100
B	1.81198000	1.70956800	0.97782200
B	1.63361200	-1.28840000	0.75860000
B	1.60991000	0.46586200	-1.58631900
B	1.21140200	-1.89639800	2.32158200
B	-0.40123100	-1.79546100	1.75140200
B	1.65607000	1.84967900	-0.66595100
B	1.15684900	1.90680400	-2.25473200
B	0.38349800	-0.70519800	2.85201600
B	0.40123100	1.79546100	1.75140200
B	-1.63361200	1.28840000	0.75860000
B	-1.15684900	-1.90680400	-2.25473200
B	-0.79495600	-2.83856900	0.43663700
B	0.27395400	2.98247900	-1.34049600
B	-1.65607000	-1.84967900	-0.66595100
B	-1.86330500	0.99269700	-0.87661400
B	-1.24310500	2.39542800	-0.54834700
B	-1.95187100	-0.27981900	0.15532200
B	1.86330500	-0.99269700	-0.87661400
B	0.52354600	0.59548300	-2.87848700
B	-0.27395400	-2.98247900	-1.34049600
B	0.91400200	-2.93418600	1.09567500