

High-Nitrogen-Content Energetic BN_n^+ ($n=4-16$) Clusters

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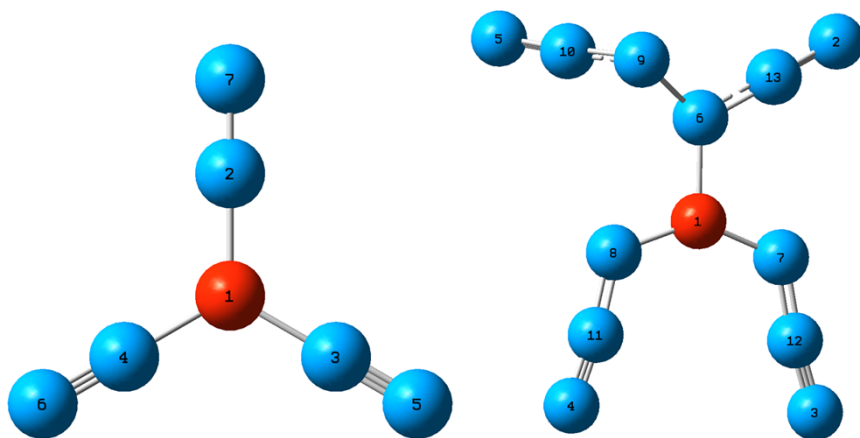


Fig. S1 The labels of B and N atom in lowest-energy structure of BN_6^+ and BN_{12}^+ cluster.

Table S1. Fuzzy bond order (FBO) and Wiberg bond order (WBO) of B-N and N-N bond in lowest-energy structure of BN_6^+ cluster.

Bond	B1-N2	B1-N3	B1-N4	N2-N7	N4-N6	N3-N5
FBO	1.09	1.09	1.09	2.74	2.74	2.74
WBO	1.16	1.16	1.16	3.11	3.11	3.11

Table S2. Fuzzy bond order (FBO) and Wiberg bond order (WBO) of B-N and N-N bond in lowest-energy structure of BN_{12}^+ cluster.

Bond	B1-N6	B1-N7	B1-N8	N6-N9	N9-N10	N10-N5	N6-N13	N13-N2	N8-N11	N11-N4	N7-N12	N12-N3
FBO	0.87	1.22	1.23	1.18	0.14	2.66	1.40	2.71	1.66	2.63	1.66	2.63
WBO	0.98	1.40	1.41	1.21	1.61	3.02	1.36	3.08	1.63	2.99	1.63	2.99