Supporting Information

**Chemisorption of pyrimidine nucleotide onto exterior surface of pristine B12N12 nanocluster: A theoretical study**

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**The optimized coordinates of all studied systems**

B12N12 in gas phase

B 0.00000000 -0.96305800 1.97870500

B 1.97870500 0.00000000 -0.96305800

B 0.00000000 -0.96305800 -1.97870500

B -1.97870500 0.00000000 -0.96305800

B -1.97870500 0.00000000 0.96305800

B -0.96305800 1.97870500 0.00000000

B 0.00000000 0.96305800 1.97870500

B 1.97870500 0.00000000 0.96305800

B 0.96305800 1.97870500 0.00000000

B 0.96305800 -1.97870500 0.00000000

B -0.96305800 -1.97870500 0.00000000

B 0.00000000 0.96305800 -1.97870500

N 0.00000000 -2.13884900 -1.13077700

N 1.13077700 0.00000000 -2.13884900

N 2.13884900 -1.13077700 0.00000000

N 0.00000000 -2.13884900 1.13077700

N -1.13077700 0.00000000 2.13884900

N -2.13884900 -1.13077700 0.00000000

N -1.13077700 0.00000000 -2.13884900

N 0.00000000 2.13884900 -1.13077700

N 2.13884900 1.13077700 0.00000000

N 1.13077700 0.00000000 2.13884900

N 0.00000000 2.13884900 1.13077700

N -2.13884900 1.13077700 0.00000000

B12N12/pyrimidine complexin gas phase

B 0.41376900 -2.11127200 1.97133100

B 1.77138700 -0.39021900 -0.94691600

B 0.41376900 -2.11127200 -1.97133100

B -1.78109100 -2.11129600 -0.96005500

B -1.78109100 -2.11129600 0.96005500

B -1.67939300 0.10392100 0.00000000

B -0.42117400 -0.37067700 1.95277800

B 1.77138700 -0.39021900 0.94691600

B 0.02887100 1.23003300 0.00000000

B 1.72551300 -2.61584200 0.00000000

B -0.01087800 -3.45418100 0.00000000

B -0.42117400 -0.37067700 -1.95277800

N 0.92699900 -3.18026800 -1.13188200

N 1.01408700 -0.75298900 -2.12941400

N 2.42473000 -1.35057200 0.00000000

N 0.92699900 -3.18026800 1.13188200

N -1.01973500 -1.73833800 2.13413900

N -1.43960700 -3.20815900 0.00000000

N -1.01973500 -1.73833800 -2.13413900

N -0.93039500 0.68798200 -1.13094900

N 1.45570700 0.69860400 0.00000000

N 1.01408700 -0.75298900 2.12941400

N -0.93039500 0.68798200 1.13094900

N -2.41168400 -1.16148200 0.00000000

C -1.14053200 3.54180000 0.00000000

C -0.12023700 5.58075000 0.00000000

C 1.14633200 4.97969000 0.00000000

C 1.18961500 3.58421300 0.00000000

N 0.04126400 2.87197400 0.00000000

H -0.22945300 6.66724900 0.00000000

H -2.03466000 2.92264800 0.00000000

H 2.06282200 5.56677700 0.00000000

H 2.10277500 2.99007800 0.00000000

N -1.26689800 4.86679200 0.00000000

B12N12 in water medium

B 0.00000000 -0.96243900 1.97508800

B 1.97508800 0.00000000 -0.96243900

B 0.00000000 -0.96243900 -1.97508800

B -1.97508800 0.00000000 -0.96243900

B -1.97508800 0.00000000 0.96243900

B -0.96243900 1.97508800 0.00000000

B 0.00000000 0.96243900 1.97508800

B 1.97508800 0.00000000 0.96243900

B 0.96243900 1.97508800 0.00000000

B 0.96243900 -1.97508800 0.00000000

B -0.96243900 -1.97508800 0.00000000

B 0.00000000 0.96243900 -1.97508800

N 0.00000000 -2.13757700 -1.13077900

N 1.13077900 0.00000000 -2.13757700

N 2.13757700 -1.13077900 0.00000000

N 0.00000000 -2.13757700 1.13077900

N -1.13077900 0.00000000 2.13757700

N -2.13757700 -1.13077900 0.00000000

N -1.13077900 0.00000000 -2.13757700

N 0.00000000 2.13757700 -1.13077900

N 2.13757700 1.13077900 0.00000000

N 1.13077900 0.00000000 2.13757700

N 0.00000000 2.13757700 1.13077900

N -2.13757700 1.13077900 0.00000000

B12N12/pyrimidine complexin water medium

B 0.41589100 -2.11039200 1.97168000

B 1.76732400 -0.38323900 -0.94584300

B 0.41589100 -2.11039200 -1.97168000

B -1.77849400 -2.11852800 -0.95969000

B -1.77849400 -2.11852800 0.95969000

B -1.67984100 0.10185800 0.00000000

B -0.42407700 -0.37003700 1.95084400

B 1.76732400 -0.38323900 0.94584300

B 0.02408500 1.25589700 0.00000000

B 1.73142500 -2.61089100 0.00000000

B -0.00332600 -3.45674500 0.00000000

B -0.42407700 -0.37003700 -1.95084400

N 0.93320700 -3.18062600 -1.13237100

N 1.01234200 -0.75344700 -2.13134000

N 2.42978000 -1.34761400 0.00000000

N 0.93320700 -3.18062600 1.13237100

N -1.01974800 -1.74466100 2.13511400

N -1.43412200 -3.21760700 0.00000000

N -1.01974800 -1.74466100 -2.13511400

N -0.93587300 0.68263900 -1.13095700

N 1.44323300 0.69287600 0.00000000

N 1.01234200 -0.75344700 2.13134000

N -0.93587300 0.68263900 1.13095700

N -2.41201800 -1.17164500 0.00000000

C -1.14295000 3.54691200 0.00000000

C -0.11729200 5.58635900 0.00000000

C 1.14703900 4.98232900 0.00000000

C 1.19025400 3.58901900 0.00000000

N 0.03900400 2.87464600 0.00000000

H -0.22138500 6.67200000 0.00000000

H -2.04057100 2.93304400 0.00000000

H 2.06334000 5.56746200 0.00000000

H 2.10913300 3.00743000 0.00000000

N -1.26587200 4.87063500 0.00000000