

## Is the planar hexacoordinate nitrogen molecule $\text{NB}_6^-$ viable?

### Supporting Information.

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The detailed Cartesian coordinates of the minimum isomers and the connected transition states obtained at B3LYP/6-311+G(d).

01

Charge = -1 Multiplicity = 1

B,0,0.,-1.5680920605,-0.0641929587

B,0,0.,0.7881131271,-1.4338836787

B,0,0.,-0.7881131271,-1.4338836787

B,0,0.,-0.8252317149,1.3552476167

B,0,0.,0.8252317149,1.3552476167

B,0,0.,1.5680920605,-0.0641929587

N,0,0.,0.,0.1425672214

State=1-A1\HF=-203.6224306

02

Charge = -1 Multiplicity = 1

N,0,-0.87868607,-0.38625067,0.

B,0,0.09806611,-0.53405418,1.28617387

B,0,0.60674164,-1.28987214,0.

B,0,0.09806611,-0.53405418,-1.28617387

B,0,0.12335808,0.98804028,-1.63691389

B,0,0.18336335,0.922816,0.

B,0,0.12335808,0.98804028,1.63691389

State=1-A\HF=-203.6364836

03

Charge = -1 Multiplicity = 1

N,0,0.,0.,0.879795

B,0,-0.78952898,-0.97121865,-0.2859374

B,0,-1.98985073,0.,-0.04349196

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B,0,1.98985073,0.,-0.04349196

B,0,0.78952898,-0.97121865,-0.2859374

B,0,-0.78952898,0.97121865,-0.2859374  
State=1-A\HF=-203.6672551

04

Charge = -1 Multiplicity = 1  
B,0,1.090381,0.983233,-0.019941  
B,0,-0.516297,1.070047,0.064204  
B,0,-0.516295,-1.070047,0.064204  
B,0,-1.617895,-0.0000001392,0.750227  
B,0,1.090382,-0.983233,-0.019942  
B,0,2.245329,0.0000001932,0.073939  
N,0,-1.268289,-0.0000001091,-0.651922  
State=1-A\HF=-203.6983351

05

B,0,-2.41879112,-0.36631652,0.  
N,0,-1.36031191,0.53790827,0.  
B,0,0.01662916,0.80129998,0.  
B,0,0.94755281,-0.75822122,0.  
B,0,2.47738687,-0.41926562,0.  
B,0,1.58312216,0.82061664,0.  
B,0,-0.70146321,-0.83118484,0.  
State=1-A\HF=-203.7616703

06

Charge = -1 Multiplicity = 1  
B,0,-0.71406886,-0.68514792,0.  
N,0,-2.10800084,-0.42778281,0.  
B,0,-1.50396675,0.80633114,0.  
B,0,0.12069426,0.96188802,0.  
B,0,1.67148925,0.7870539,0.  
B,0,2.48181215,-0.52478617,0.  
B,0,0.89524113,-0.74644304,0.  
State=1-A\HF=-203.8030996

Ts01/02

Charge = -1 Multiplicity = 1  
B,0,1.5493798156,0.6249968433,-0.1117840197  
B,0,1.2292430478,-0.9062821887,-0.1109392547  
B,0,-0.2947055847,-1.5527245204,-0.230642728  
B,0,-1.4742879074,-0.4146311759,0.0265758988  
B,0,-1.2336305111,1.1310936178,0.0281035197  
N,0,-0.0337765785,-0.3121639432,0.451669656  
B,0,0.2712883497,1.5545769443,-0.2336509345

State=1-A\HF=-203.6130961

Ts02/03

Charge = -1 Multiplicity = 1

N,0,-0.2972859195,-0.8773317982,-0.2842343002  
B,0,-0.3046100718,-0.5835534862,1.32022236  
B,0,1.1149672117,-0.5610737588,0.6640727011  
B,0,1.0555052913,-0.1048228514,-0.8459084047  
B,0,0.3110645444,1.0063553492,-1.6577986905  
B,0,-0.4905262133,0.8037731815,-0.2432286162  
B,0,-1.3600863655,0.5324007265,1.0991048801

State=1-A\HF=-203.6361088

Ts03/04

Charge = -1 Multiplicity = 1

N,0,0.1611848305,-0.1185548668,1.0077409671  
B,0,0.7967951737,-1.0160482079,-0.1844265653  
B,0,-0.7427784127,-0.9128929728,-0.5615664431  
B,0,-0.7821657491,0.9895309907,-0.3279576125  
B,0,-1.9878654498,0.0243382136,-0.5365886333  
B,0,0.7547704866,1.062045195,0.0675131265  
B,0,1.8346470258,-0.0073315723,0.3690138334

State=1-A\HF=-203.6616642

Ts04/05

Charge = -1 Multiplicity = 1

N,0,-1.2336607485,0.2494143762,0.8317155008  
B,0,1.0722077767,0.9498221651,-0.5001762419  
B,0,2.1555106928,-0.1031554171,-0.4930701196  
B,0,1.0188356532,-0.9096930455,0.1217666755  
B,0,-0.5664143022,-1.0174145896,0.3751779794  
B,0,-0.4249825369,1.0268451015,-0.0318402951  
B,0,-1.9139038259,-0.2399219864,-0.3552767936

State=1-A\HF=-203.6907093

Ts05/06

Charge = -1 Multiplicity = 1

B,0,2.0105345173,-0.3481925757,0.3783199985  
N,0,1.5821276804,0.7448771125,-0.2367106681  
B,0,0.1700264991,0.7038804019,0.0412445904  
B,0,-0.9129136283,-0.715757423,-0.1342944588  
B,0,-2.4206095078,-0.2475200455,0.0414854331  
B,0,-1.387730493,0.8929983294,0.1818875308  
B,0,0.6240660936,-1.1829670867,-0.1941885732

State=1-A\HF=-203.7254796

X01

Charge = 0 Multiplicity = 1

B,0,0.,1.599655,1.514967  
B,0,-1.3853418673,0.7998275,1.514967  
B,0,1.3853418673,0.7998275,1.514967  
N,0,0.,0.,1.95136  
B,0,-1.3853418673,-0.7998275,1.514967  
B,0,1.3853418673,-0.7998275,1.514967  
B,0,0.,-1.599655,1.514967  
Fe,0,0.,0.,0.  
B,0,1.599655,0.,-1.514967  
B,0,0.7998275,-1.3853418673,-1.514967  
B,0,0.7998275,1.3853418673,-1.514967  
N,0,0.,0.,-1.95136  
B,0,-0.7998275,-1.3853418673,-1.514967  
B,0,-0.7998275,1.3853418673,-1.514967  
B,0,-1.599655,0.,-1.514967

State=1-A1\HF=-1670.9572851

X02

Charge = 0 Multiplicity = 1

B,0,-1.1525628697,1.2924465797,-1.2522815529  
B,0,-0.8549954212,1.7258315197,1.2463229929  
B,0,-0.9341769326,0.427654203,2.0890110197  
B,0,-1.2576977089,-1.0120814529,1.7202918551  
B,0,-1.6179307739,-1.6070481934,0.3405787805  
N,0,-1.2852477767,0.0586156732,-1.6251331079  
B,0,-1.2452352453,-1.3240869613,-1.1997964871  
N,0,1.8094107962,-0.1827172527,-0.8046391446  
B,0,0.2127483124,-1.9504374019,-1.0361299736  
B,0,0.9178421963,1.961698934,0.0720803102  
B,0,-0.5712400179,2.3443704705,-0.1770573683  
B,0,1.623378438,-1.5911953814,-0.4024410709  
B,0,2.4445211191,-0.6484626623,0.5947687264  
B,0,2.0590728323,0.8569242979,0.2026921386  
Fe,0,-0.0985928909,-0.0445542327,0.1808867021

State=1-A\HF=-1671.2576737

Tsx01/x02

Charge = 0 Multiplicity = 1

B,0,-0.881073,1.719481,-0.000057

B,0,-1.387595,0.901633,1.320699  
B,0,-1.633506,-0.680803,1.392581  
B,0,-1.748305,-1.474121,0.00004  
B,0,-1.633679,-0.680778,-1.392521  
N,0,-1.964372,0.129851,-0.00003  
B,0,-1.387738,0.901611,-1.320708  
N,0,1.944366,0.181092,0.000012  
B,0,1.338278,1.360754,-0.82671  
B,0,1.511199,-0.057078,1.575309  
B,0,1.338009,1.361277,0.825915  
B,0,1.511381,-0.058065,-1.575288  
B,0,1.51305,-1.451805,-0.798505  
B,0,1.513,-1.451296,0.799259  
Fe,0,-0.00481,-0.158872,0.000002  
State=1-A\HF=-1670.9482091