

Supporting Information

Adsorption of Phosgene Gas on Pristine and Copper Decorated B₁₂N₁₂ Nanocages: A Comparative DFT Study

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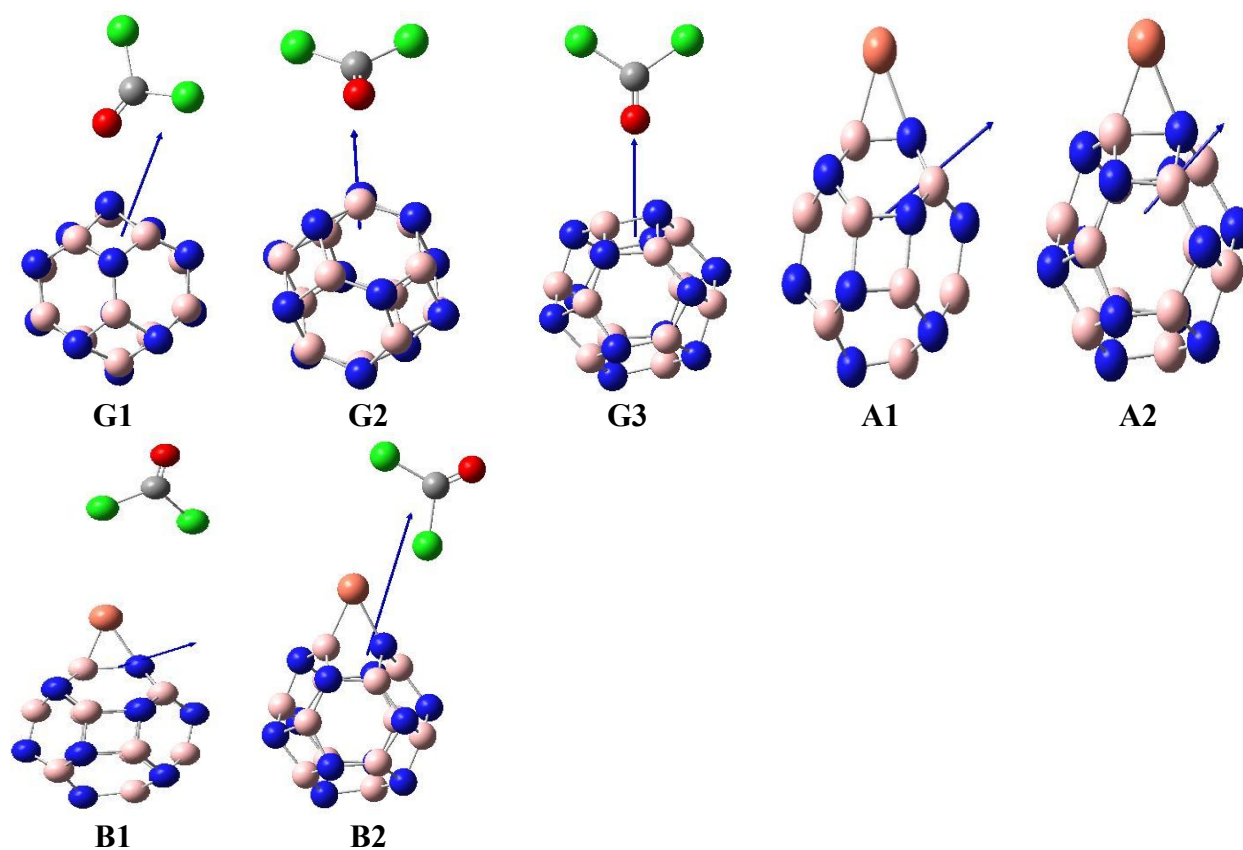


Figure S1. Dipole moment vector representation in all systems

Optimized Cartesian coordinate of all geometries

$B_{12}N_{12}$ nanocage

Symbol	X	Y	Z
N	0.69093600	-2.16480000	0.78377400

N	-0.55934300	-0.45081400	2.29354100
N	1.89574100	-0.38117200	1.42836800
N	-1.92711100	0.89529600	1.12466200
N	0.48228100	1.80454600	1.51282600
N	-0.69093700	2.16483600	-0.78381900
N	-1.89580500	0.38115000	-1.42835200
N	-1.79706800	-1.56970200	0.29411300
N	1.92700200	-0.89523600	-1.12459400
N	0.55944500	0.45077400	-2.29353000
N	-0.48230200	-1.80451300	-1.51286700
N	1.79706100	1.56971400	-0.29412500
B	-0.47124900	-2.13790800	-0.06456600
B	-1.66677300	-0.55662600	1.30785600
B	-1.63992700	-0.98734000	-1.06450600
B	0.63663200	-0.96811800	-1.85819500
B	-1.75981400	1.27947300	-0.25195300
B	-0.63615800	1.07840800	-1.79651100
B	0.47124200	2.13790300	0.06450900
B	1.66683500	0.55666400	-1.30788000
B	-0.63662800	0.96810700	1.85811600
B	1.63990100	0.98735400	1.06451600
B	1.75985500	-1.27953200	0.25204300
B	0.63622400	-1.07849600	1.79657600

G1

Symbol	X	Y	Z
N	3.46509900	0.18284800	-1.39123500
N	1.29171900	-1.03405000	-2.15219700
N	3.05084500	-1.78187300	-0.38245200
N	-0.55776900	-0.16458700	-1.21718000
N	0.51291100	-2.16337700	0.06239100
N	-0.44887700	-0.13698000	1.38513500
N	-0.03474000	1.82589600	0.37609700
N	1.29619300	1.55240000	-1.84489300
N	3.57611200	0.21035500	1.21073900
N	1.72616500	1.07915200	2.14485300
N	2.50305300	2.20982800	-0.06791000
N	1.72036600	-1.50630600	1.83951100
B	2.66057200	1.37247300	-1.28536900
B	0.62738400	0.28629100	-1.98741900
B	1.07824800	2.11318400	-0.48526100
B	2.74276400	1.43848300	1.12278100
B	-0.65303800	0.50900200	0.05689800
B	0.40399800	1.06403200	1.57136100
B	0.35482600	-1.32288700	1.27904400
B	2.38885700	-0.24027500	1.98355400
B	0.27414600	-1.38940400	-1.12784400
B	1.93543800	-2.06842900	0.48111500
B	3.64448800	-0.45711900	-0.06223000
B	2.61223000	-1.01996000	-1.58147900

C	-4.13778600	0.23848800	0.04072400
Cl	-5.81479500	0.76168500	-0.05543000
Cl	-3.97476800	-1.50944200	0.01105900
O	-3.22597800	0.99260600	0.11802600

G2

Symbol	X	Y	Z
N	-3.13552900	1.42608300	-1.02767200
N	-2.09452100	1.90664500	1.31077600
N	-3.80113800	0.06127300	0.62834200
N	0.00067200	1.11764600	1.50210300
N	-1.88329500	-0.49280400	2.30048800
N	0.16155700	-1.42830100	0.98925200
N	0.83049700	-0.06509900	-0.66633600
N	-0.62436100	2.08855500	-0.83145700
N	-2.97473100	-1.12253400	-1.53977100
N	-0.87907400	-1.91035500	-1.34773500
N	-1.08992000	0.48807800	-2.33817300
N	-2.34865400	-2.09390100	0.79433000
B	-1.79879400	1.52989700	-1.55018800
B	-0.79396700	1.98241300	0.59440800
B	-0.00839300	0.85530500	-1.38647400
B	-1.61021600	-0.82125800	-2.04572400
B	0.55955500	-0.00839500	0.79966200
B	0.14830700	-1.37478200	-0.49334000

B	-1.17335500	-1.53370000	1.51289600
B	-2.17862400	-1.98836600	-0.63051000
B	-1.36220700	0.81655900	2.00843300
B	-2.96490400	-0.86078900	1.35056800
B	-3.52133500	0.00434200	-0.83030200
B	-3.12232700	1.37265900	0.45792700
C	4.13239400	-0.00759200	0.42989600
Cl	4.82529600	-1.44173700	-0.32166000
Cl	4.72326300	1.48212900	-0.29870200
O	3.36011300	-0.04219400	1.32637100

G3

Symbol	X	Y	Z
N	1.36350300	1.47776600	1.86545300
N	-0.16250700	-0.58685700	1.43483200
N	-0.05643000	1.66738700	0.13508700
N	0.90648300	-2.25047200	0.37039800
N	-0.36069900	-0.57048500	-1.16259400
N	1.97203100	-1.47929000	-1.87764900
N	3.39275000	-1.66928500	-0.14748300
N	2.32747500	-0.92985300	2.11019500
N	2.42830200	2.24843400	-0.38343400
N	3.50038900	0.58508400	-1.44755700
N	3.69766000	0.56913900	1.14942900
N	1.00852400	0.92885200	-2.12319800

B	2.45344400	0.54359900	1.96307800
B	1.07472200	-1.39421200	1.57361400
B	3.37142700	-0.87795400	1.05452800
B	3.47586700	1.23062300	-0.10907400
B	2.02049000	-2.09824400	-0.52695000
B	3.19291400	-0.81772200	-1.34909200
B	0.88174100	-0.54451800	-1.97470100
B	2.26044500	1.39328400	-1.58725800
B	-0.14491400	-1.23215200	0.09734700
B	-0.03782500	0.87624500	-1.06654200
B	1.31362100	2.09583000	0.51471500
B	0.13991200	0.81598400	1.33700600
C	-4.51196900	-0.00646300	0.11404900
Cl	-5.50386700	-1.45294800	-0.07506700
Cl	-5.45162500	1.47485100	-0.07214100
O	-3.35205100	-0.02754000	0.34006700

A1

Symbol	X	Y	Z
N	0.07825700	0.79528100	-2.13010800
N	-2.26163000	1.40504900	-1.15057300
N	-1.43178300	-0.86726600	-2.10476400
N	-2.26311600	1.44498800	1.09822500
N	-2.94738600	-0.82208500	0.01358100
N	-1.43347000	-0.79156400	2.13372900

N	0.07613800	0.87100500	2.10133700
N	-0.09651200	2.31905900	-0.04114600
N	0.89256700	-1.45252100	-1.09811100
N	0.89171800	-1.41237900	1.14946200
N	1.61152300	0.86545800	-0.01437800
N	-1.27907500	-2.32910300	0.04145100
B	0.63830200	1.45213800	-0.98949400
B	-1.50886300	2.02750900	-0.03641000
B	0.63693900	1.48733500	0.93833500
B	1.56512700	-0.68256300	0.01288100
B	-1.39360500	0.67707900	1.95248900
B	0.03652600	-0.61407500	1.96282900
B	-2.00475900	-1.44211400	0.98389000
B	0.13201900	-2.02054000	0.03590800
B	-2.79275600	0.60575700	-0.01178300
B	-2.00406500	-1.47686200	-0.93272600
B	0.03822300	-0.68433400	-1.94032500
B	-1.39109400	0.60663400	-1.97494600
Cu	3.35791000	0.00478400	0.00020100

A2

Symbol	X	Y	Z
N	-1.61854300	0.89848100	0.09177700
N	0.22371200	1.47774400	1.82203100
N	-0.99131100	-0.78841100	1.51422900

N	2.30758000	1.47602700	0.97923800
N	1.54446600	-0.73920700	2.11689300
N	2.93985200	-0.81578100	-0.08154700
N	2.35158100	0.79386600	-1.53553100
N	0.44129000	2.31112700	-0.63096600
N	-0.94065200	-1.49301200	-0.97499600
N	1.13345800	-1.48519700	-1.83337800
N	-0.19709900	0.73775400	-2.10004400
N	0.92743300	-2.30601200	0.63139600
B	-0.72219900	1.43574800	-0.90474600
B	0.97506700	2.05752600	0.68047500
B	1.05291600	1.39997400	-1.63330800
B	-0.12447400	-0.69049600	-1.90201900
B	2.76725900	0.65831000	-0.11318700
B	2.23491000	-0.68140800	-1.38437100
B	2.08333800	-1.41661500	0.90897200
B	0.39098700	-2.05883900	-0.68052000
B	1.47490200	0.68102900	1.92063900
B	0.30295800	-1.39797500	1.62562300
B	-1.56639300	-0.76560600	0.12036500
B	-0.87588200	0.66792300	1.36649400
Cu	-3.33859700	0.00277500	-0.00054500

B1

Symbol	X	Y	Z
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N	1.17735500	-0.07092300	2.17389600
N	3.51332100	1.05864200	1.89323700
N	2.90392700	-1.46941000	1.84564400
N	3.80849200	1.91153600	-0.16667600
N	4.66645000	-0.52417400	0.17552700
N	3.46103900	0.13841400	-2.03707700
N	1.73332500	1.53408400	-1.70300900
N	1.40508400	2.11507600	0.80119000
N	0.84591400	-1.85439900	0.30477600
N	1.14181100	-1.00219400	-1.75418900
N	-0.05501600	0.62566200	-0.02449200
N	3.25475900	-2.06016500	-0.66288500
B	0.68424500	0.90242500	1.24823700
B	2.83254700	1.97310000	0.94688400
B	0.93874600	1.63249100	-0.51766800
B	0.22000800	-0.79768500	-0.57440000
B	3.18244200	1.43170100	-1.37292400
B	1.97167700	0.10919900	-2.07797100
B	3.96293300	-0.83161300	-1.09892000
B	1.82552000	-1.90179100	-0.80206100
B	4.30179500	0.77723800	0.66175100
B	3.71023600	-1.55828600	0.65650000
B	1.45846800	-1.37102700	1.49666700
B	2.66614200	-0.05853100	2.22566400
Cu	-1.63657600	-0.33025000	-0.65493700

C	-6.46450400	0.16185600	0.18618000
O	-7.63658600	0.30070700	0.17768400
Cl	-5.65031000	-1.39324000	0.36709900
Cl	-5.31607700	1.50202400	0.01962000

B2

Symbol	X	Y	Z
N	-0.38298800	-0.35685000	-0.29163200
N	1.40274500	-1.23136300	-1.95381400
N	0.76103900	1.23420700	-1.50077200
N	3.35017300	-1.82498900	-0.99858900
N	3.24693800	0.59533800	-1.95745800
N	4.43744500	0.14340700	0.31483000
N	3.35596700	-1.37581000	1.56931200
N	1.21163300	-2.28758300	0.41208700
N	0.78489800	1.70592900	1.04276300
N	2.71803100	1.10643700	2.01718400
N	0.86191700	-0.72243400	1.98382500
N	2.91728300	2.14545600	-0.36609100
B	0.28082700	-1.16908500	0.69641000
B	1.89509800	-2.07239400	-0.83523600
B	1.94396000	-1.63984600	1.53119900
B	1.30043600	0.65370200	1.92908600
B	3.90580800	-1.23726900	0.19347800
B	3.61722300	0.08889200	1.55503600

B	3.83549500	1.01816900	-0.66034800
B	2.23083300	1.93721400	0.88211700
B	2.81488500	-0.77178000	-1.90234900
B	2.16711700	1.50410800	-1.47705400
B	0.05736100	1.27948700	-0.15541400
B	0.50354400	-0.20684200	-1.48189500
Cu	-1.84381500	0.93249800	-0.18578200
C	-5.38041700	-0.74542400	0.04455500
O	-6.10038300	-1.67713100	0.03475200
Cl	-3.59388500	-0.92347200	-0.13086300
Cl	-5.86860400	0.92365800	0.22296200