

## Supporting Information

### Designing Novel Zn decorated Inorganic B<sub>12</sub>P<sub>12</sub> Nanoclusters with promising electronic properties. A step forward towards efficient CO<sub>2</sub> sensing materials

Shahid Hussain<sup>a</sup>, Shahzad Ali Shahid Chatha<sup>a</sup>, Abdullah Ijaz Hussain<sup>a</sup>, Riaz Hussain<sup>b</sup>, Muhammad Yasir Mehboob<sup>b</sup>, Tahsin Gulzar<sup>a</sup>, Asim Mansha<sup>c</sup>, Nabeel Shahzad<sup>c</sup> and Khurshid Ayub<sup>d</sup> \*.

<sup>a</sup> Department of Applied Chemistry, Government College University, Faisalabad – 38000, Pakistan.

<sup>b</sup> Department of Chemistry, University of Okara, Okara, Punjab, Pakistan.

<sup>c</sup> Department of Chemistry, Government College University, Faisalabad – 38000, Pakistan.

<sup>d</sup> Department of Chemistry, COMSATS University, Abbottabad Campus, Abbottabad-22060, Pakistan

#### Corresponding Author

Tel: +92-992-383591

Fax: +92-992-383441

Email: [Khurshid@cuiatd.edu.pk](mailto:Khurshid@cuiatd.edu.pk) (K.A)

#### Optimized Cartesian coordinate of all geometries

##### B<sub>12</sub>P<sub>12</sub> nanocage

Symbol	X	Y	Z
B	1.18782709	2.43305319	-0.00049500
B	0.00000000	1.18828809	-2.43288118
B	-1.18782709	2.43305319	-0.00049500
B	0.00000000	1.18790509	2.43364818
B	-2.43299318	0.00000000	-1.18798909
B	-2.43290519	0.00000000	1.18794809
B	-1.18782709	-2.43305319	-0.00049500
B	-0.00000000	-1.18790509	2.43364818
B	-0.00000000	-1.18828809	-2.43288118
B	1.18782709	-2.43305319	-0.00049500
B	2.43290519	-0.00000000	1.18794809

## Supporting Information

B	2.43299318	-0.00000000	-1.18798909
P	-2.83481622	1.46638211	0.00016400
P	-2.83481622	-1.46638211	0.00016400
P	-1.46619511	0.00000000	-2.83481122
P	0.00000000	2.83573622	-1.46682111
P	0.00000000	2.83424822	1.46608611
P	1.46619511	-0.00000000	-2.83481122
P	2.83481622	1.46638211	0.00016400
P	2.83481622	-1.46638211	0.00016400
P	1.46652111	-0.00000000	2.83530621
P	-1.46652111	0.00000000	2.83530621
P	-0.00000000	-2.83424822	1.46608611
P	-0.00000000	-2.83573622	-1.46682111

### CO<sub>2</sub>-B<sub>12</sub>P<sub>12</sub>

Symbol	X	Y	Z
B	0.64857300	2.28844900	0.84326600
B	-1.12707400	0.62887000	2.57064300
B	1.65187300	0.25295600	1.56165600
B	1.69090000	0.61865100	-1.39721600
B	-0.20379400	-2.06923400	1.70440700
B	1.17454400	-2.07546800	-0.23327800
B	-1.73862500	-2.27313700	-0.84276900
B	0.03619200	-0.61607700	-2.56930100
B	-2.78281100	-0.60600900	1.39637800
B	-2.74319000	-0.24190700	-1.56088500

## Supporting Information

B	-0.88551200	2.08412900	-1.70424200
B	-2.26229300	2.08849700	0.23360900
P	1.67686400	-1.65525100	1.58091700
P	-0.36786800	-3.17666300	0.13272900
P	-1.56772300	-1.24049300	2.75407900
P	0.58119700	1.48177200	2.59482300
P	2.27839400	1.47534000	0.20579000
P	-2.80782800	1.26504200	1.86804100
P	-0.72202100	3.19183900	-0.13254200
P	-2.76571500	1.66770100	-1.58083500
P	0.47634200	1.25406500	-2.75466100
P	1.71790200	-1.25072500	-1.86799600
P	-1.67219700	-1.46903300	-2.59550000
P	-3.37031300	-1.46359700	-0.20539700
C	5.94776200	-0.07139800	-0.00001800
O	5.08932900	-0.86698100	-0.00859400
O	6.80617300	0.72070300	0.00822300

### D1

Symbol	X	Y	Z
B	1.18782700	2.43305300	-0.00049500
B	0.00000000	1.18828800	-2.43288100
B	-1.18782700	2.43305300	-0.00049500
B	0.00000000	1.18790500	2.43364800
B	-2.43299300	0.00000000	-1.18798900
B	-2.43290500	0.00000000	1.18794800

## Supporting Information

B	-1.18782700	-2.43305300	-0.00049500
B	0.00000000	-1.18790500	2.43364800
B	0.00000000	-1.18828800	-2.43288100
B	1.18782700	-2.43305300	-0.00049500
B	2.43290500	0.00000000	1.18794800
B	2.43299300	0.00000000	-1.18798900
P	-2.83481600	1.46638200	0.00016400
P	-2.83481600	-1.46638200	0.00016400
P	-1.46619500	0.00000000	-2.83481100
P	0.00000000	2.83573600	-1.46682100
P	0.00000000	2.83424800	1.46608600
P	1.46619500	0.00000000	-2.83481100
P	2.83481600	1.46638200	0.00016400
P	2.83481600	-1.46638200	0.00016400
P	1.46652100	0.00000000	2.83530600
P	-1.46652100	0.00000000	2.83530600
P	0.00000000	-2.83424800	1.46608600
P	0.00000000	-2.83573600	-1.46682100
Zn	0.91754779	-0.73920798	2.79677697

## D2

Symbol	X	Y	Z
B	1.02554058	2.38253919	1.26672008
B	-0.16228642	1.13777419	-1.16566592
B	-1.35011342	2.38253919	1.26672008
B	-0.16228642	1.13739119	3.70086308

## Supporting Information

B	-2.59527942	-0.05051381	0.07922608
B	-2.59519142	-0.05051381	2.45516308
B	-1.35011342	-2.48356681	1.26672008
B	-0.16228642	-1.23841881	3.70086308
B	-0.16228642	-1.23880181	-1.16566592
B	1.02554058	-2.48356681	1.26672008
B	2.27061858	-0.05051381	2.45516308
B	2.27070658	-0.05051381	0.07922608
P	-2.99710242	1.41586819	1.26737908
P	-2.99710242	-1.51689581	1.26737908
P	-1.62848142	-0.05051381	-1.56759592
P	-0.16228642	2.78522219	-0.19960592
P	-0.16228642	2.78373419	2.73330108
P	1.30390858	-0.05051381	-1.56759592
P	2.67252958	1.41586819	1.26737908
P	2.67252958	-1.51689581	1.26737908
P	1.30423458	-0.05051381	4.10252108
P	-1.62880742	-0.05051381	4.10252108
P	-0.16228642	-2.88476181	2.73330108
P	-0.16228642	-2.88624981	-0.19960592
Zn	0.62145805	-0.71647923	-3.15801940

### D3

Symbol	X	Y	Z
B	1.18782700	2.43305300	-0.00049500
B	0.00000000	1.18828800	-2.43288100

## Supporting Information

B	-1.18782700	2.43305300	-0.00049500
B	0.00000000	1.18790500	2.43364800
B	-2.43299300	0.00000000	-1.18798900
B	-2.43290500	0.00000000	1.18794800
B	-1.18782700	-2.43305300	-0.00049500
B	0.00000000	-1.18790500	2.43364800
B	0.00000000	-1.18828800	-2.43288100
B	1.18782700	-2.43305300	-0.00049500
B	2.43290500	0.00000000	1.18794800
B	2.43299300	0.00000000	-1.18798900
P	-2.83481600	1.46638200	0.00016400
P	-2.83481600	-1.46638200	0.00016400
P	-1.46619500	0.00000000	-2.83481100
P	0.00000000	2.83573600	-1.46682100
P	0.00000000	2.83424800	1.46608600
P	1.46619500	0.00000000	-2.83481100
P	2.83481600	1.46638200	0.00016400
P	2.83481600	-1.46638200	0.00016400
P	1.46652100	0.00000000	2.83530600
P	-1.46652100	0.00000000	2.83530600

### D4

Symbol	X	Y	Z
B	-1.25486100	2.59451800	-0.52474400
B	-2.85567000	0.91074100	1.34176800
B	-0.16018900	2.16493200	1.54029400

## Supporting Information

B	1.45520800	1.40743300	-0.84295200
B	-0.61705000	-0.56377000	2.64640100
B	1.48523600	-0.31750100	1.57502200
B	-0.11962400	-2.59592100	0.52524600
B	1.47450900	-0.90620100	-1.33667600
B	-2.83587100	-1.41385200	0.84599000
B	-1.21464700	-2.16382900	-1.53927700
B	-0.75543400	0.56437500	-2.64889300
B	-2.86403900	0.31811500	-1.57813600
P	0.61012100	0.92057100	2.76747300
P	0.63465100	-1.94828700	2.15598300
P	-2.52418400	-0.55890100	2.54756700
P	-2.01182900	2.62119900	1.24997500
P	0.59113400	2.92321000	-0.06709000
P	-3.87949600	-0.02755400	0.00201200
P	-2.00696500	1.94745600	-2.15636700
P	-1.98250900	-0.91955500	-2.76757000
P	1.15375000	0.55931600	-2.54888300
P	2.49623000	0.02688000	-0.00054100
P	0.63792500	-2.62038900	-1.24925100
P	-1.96476600	-2.92421300	0.06761100
Zn	5.50004100	0.00029300	-0.00113300

### E1

Symbol	X	Y	Z
B	0.36492700	-2.78876800	0.02409600

## Supporting Information

B	2.82405700	-1.19911100	-0.63055600
B	1.36301100	-1.67791400	1.89256300
B	-1.65677300	-1.10338300	1.35549100
B	2.58936700	1.00050900	1.38949400
B	0.46452500	1.07803600	2.27762700
B	0.68886900	2.85772300	-0.06391900
B	-2.09239000	1.77203700	0.57704500
B	2.43944300	0.93466400	-1.57476900
B	-0.49940900	1.77456400	-1.69306900
B	-1.75697700	-1.36917100	-1.17934200
B	0.46653800	-1.12240700	-2.32015600
P	1.88416900	-0.09307800	2.81297700
P	1.49889100	2.56977500	1.64247700
P	3.63044400	0.48536900	-0.13235100
P	2.24242600	-2.64015100	0.48320100
P	-0.38082100	-2.49402400	1.78337400
P	2.33684100	-0.77622500	-2.45375700
P	-0.44967500	-2.71734100	-1.70369400
P	-1.03886400	0.05397500	-2.33290600
P	-3.09813400	-1.72115300	0.16316000
P	-1.37103200	0.71415600	1.96898200
P	-1.19490400	3.07663800	-0.45286600
P	1.31677300	2.46041900	-1.81696700
Zn	-3.55392200	0.51469100	0.01010200
C	-6.18347940	1.32283438	0.15381464



## Supporting Information

O -7.21193130 1.86409293 0.28129645

O -5.15502749 0.78157582 0.02633283

### E2

Symbol	X	Y	Z
B	-1.66090000	2.17775600	1.18939700
B	1.06534800	2.12769400	0.00537800
B	-1.66073500	2.18401900	-1.17821000
B	-3.28311000	-0.01943500	-0.00026400
B	0.49726700	0.52798400	-2.40889900
B	-1.63491100	-0.52171600	-2.43199100
B	0.50707700	-2.16678600	-1.18622400
B	-2.21779100	-2.14663400	-0.00570000
B	2.39457500	0.00759700	0.00025300
B	0.50686000	-2.17296900	1.17506000
B	-1.63514600	-0.53437700	2.42920100
B	0.49678000	0.51536700	2.41184400
P	-1.21611800	1.32013300	-2.82063900
P	0.08232400	-1.30506800	-2.83378600
P	1.96026400	1.27378600	-1.46170100
P	-0.52445800	3.19517700	0.00828600
P	-3.15607900	1.88806600	0.00472700
P	1.95947200	1.26600800	1.46816900
P	-1.21655800	1.30550000	2.82750800
P	0.08200100	-1.31986000	2.82714700
P	-3.11065600	-1.26693300	1.46271500

## Supporting Information

P	-3.11059500	-1.25938700	-1.46965900
P	-0.62305800	-3.19894000	-0.00835000
P	1.99278000	-1.89660500	-0.00475600
Zn	4.54445400	0.00264400	0.00019400
C	6.04384582	-0.05489435	-0.00023104
O	6.04384582	-0.05489435	1.16892496
O	6.04384582	-0.05489435	-1.16938704

### E3

Symbol	X	Y	Z
B	-0.56248300	2.42607800	-0.15026100
B	0.57502800	1.31708700	2.36527800
B	1.80907400	2.43342100	-0.10531100
B	0.66922900	1.06037300	-2.49113100
B	3.02876500	0.06352000	1.23237700
B	3.07522400	-0.06030100	-1.13971900
B	1.80716300	-2.43163300	0.15035700
B	0.66877100	-1.31672400	-2.36538200
B	0.57463500	-1.06078300	2.49104100
B	-0.56440500	-2.42788700	0.10521500
B	-1.77998500	-0.06361400	-1.22660700
B	-1.83039800	0.06042000	1.13851600
P	3.45380000	1.46636000	-0.02234800
P	3.45277700	-1.46271800	0.13078100
P	2.03078100	0.15031600	2.85795900
P	0.59356900	2.91233600	1.31520300

## Supporting Information

P	0.64979200	2.75679700	-1.61380900
P	-0.89840900	0.14777800	2.79828700
P	-2.21096700	1.46007000	-0.12986000
P	-2.21215100	-1.46380700	0.02367100
P	-0.78963200	-0.15010800	-2.85302600
P	2.14060400	-0.14801400	-2.80249500
P	0.64761100	-2.91204900	-1.31539700
P	0.59174000	-2.75712900	1.61363700
Zn	-4.96986000	0.00009000	-0.00203200
C	-7.83204042	1.05706380	0.60442242
O	-7.76155140	2.04136661	1.23140329
O	-7.90252945	0.07276098	-0.02255846

### E4

Symbol	X	Y	Z
B	-1.92998300	-1.39339900	2.26428300
B	-3.50972000	-1.68885000	-0.24536400
B	-0.78602900	-2.59045200	0.55936200
B	0.74687700	-0.26770300	1.61662200
B	-1.26380300	-1.58198000	-2.20318900
B	0.81231700	-0.88777000	-1.28892200
B	-0.86441200	1.36939200	-2.26942900
B	0.70817000	1.65793100	0.24125300
B	-3.54771800	0.24466700	-1.62682800
B	-2.00883600	2.56460100	-0.56306800
B	-1.52941500	1.55908700	2.20160700

## Supporting Information

B	-3.61131100	0.86460800	1.28682100
P	-0.00563100	-2.63119800	-1.18323800
P	-0.05266000	-0.24481300	-2.88838200
P	-3.17259700	-1.57654200	-2.14205500
P	-2.63609300	-2.74582800	1.08332700
P	-0.06610200	-1.89095800	2.20741200
P	-4.58832000	-0.10212500	-0.03926900
P	-2.73997000	0.22110600	2.88381700
P	-2.78710600	2.60626400	1.18010500
P	0.38159700	1.55249100	2.13875200
P	1.78435700	0.07681700	0.03355700
P	-0.15776900	2.72058500	-1.08715800
P	-2.72735600	1.86651000	-2.21212300
Zn	4.76384600	0.28326700	0.04029300
C	8.74844600	-0.25098100	-0.03153100
O	8.53702100	-1.40070100	-0.00091800
O	8.96648400	0.89727100	-0.06240000

.....