

## Supplementary materials for the manuscript “Theoretical modeling of B<sub>12</sub>N<sub>12</sub> nanocage for the effective removal of paracetamol from drinking water”

**Table S1.** Grimme's dispersion energy of the complexes.

COMPLEXES	GRIMME'S DISPERSION ENERGY
CMP-1	-0.0678366923 au
CMP-2	-0.0622449728 au
CMP-3	-0.0664845956 au

### Coordinates of CMP-1

C 6.0 -3.16676 2.26016 2.73258  
C 6.0 -3.25033 0.96791 2.19240  
C 6.0 -3.48674 -0.11759 3.04724  
C 6.0 -3.65589 0.10532 4.41086  
C 6.0 -3.58925 1.39798 4.94126  
C 6.0 -3.33640 2.48127 4.09185  
O 8.0 -3.75150 1.66898 6.26531  
H 1.0 -3.93614 0.85304 6.74575  
N 7.0 -3.07791 0.85233 0.77955  
C 6.0 -3.10149 -0.23122 -0.00254  
H 1.0 -2.93961 1.73223 0.30318  
O 8.0 -3.28509 -1.35706 0.54019  
C 6.0 -2.92006 -0.05737 -1.47986  
H 1.0 -2.75108 0.97977 -1.76827  
H 1.0 -3.81434 -0.45547 -1.97636  
H 1.0 -2.08236 -0.68918 -1.79243  
H 1.0 -2.96738 3.10762 2.07747  
H 1.0 -3.25911 3.47934 4.51380  
H 1.0 -3.54157 -1.13098 2.66981  
H 1.0 -3.84056 -0.74228 5.06682  
N 7.0 -3.32563 -3.71383 1.17476  
N 7.0 -3.38660 -5.93161 1.55222  
B 5.0 -4.30130 -4.80182 1.20624

B 5.0 -2.41737 -4.85885 1.17204  
B 5.0 -3.31897 -2.80382 -0.03098  
B 5.0 -3.43702 -6.94335 0.53939  
N 7.0 -5.49613 -4.90350 0.40267  
N 7.0 -1.26064 -5.03606 0.32632  
N 7.0 -2.21731 -3.09014 -1.11769  
B 5.0 -1.43522 -4.26784 -0.93616  
B 5.0 -1.46975 -6.16377 -0.61345  
N 7.0 -2.33947 -7.29679 -0.40383  
N 7.0 -4.58777 -7.22564 -0.36296  
B 5.0 -5.39231 -6.04025 -0.54245  
B 5.0 -5.31849 -4.14440 -0.86593  
N 7.0 -4.46840 -3.01950 -1.07827  
B 5.0 -3.37132 -3.40936 -1.97257  
N 7.0 -1.30961 -5.41763 -1.88703  
B 5.0 -3.48131 -7.26644 -1.35380  
N 7.0 -5.55063 -5.28395 -1.81015  
B 5.0 -4.40609 -5.46885 -2.65890  
N 7.0 -3.48503 -6.63855 -2.65045  
B 5.0 -2.49418 -5.52767 -2.69348  
N 7.0 -3.42246 -4.41783 -3.01616

### **Coordinates of CMP-2**

C 6.0 -6.01884 3.03077 -0.14610  
C 6.0 -4.65222 3.33117 -0.02285  
C 6.0 -3.71808 2.29049 -0.12701  
C 6.0 -4.15599 0.98308 -0.34711  
C 6.0 -5.51994 0.68692 -0.46429  
C 6.0 -6.45047 1.72900 -0.36282  
O 8.0 -6.00451 -0.56753 -0.68054  
H 1.0 -5.28462 -1.22339 -0.67155  
N 7.0 -4.30197 4.68442 0.20264  
C 6.0 -3.05825 5.23999 0.38353  
H 1.0 -5.08427 5.32077 0.24541  
O 8.0 -2.00918 4.60817 0.36653  
C 6.0 -3.06632 6.74710 0.61579  
H 1.0 -4.06250 7.20307 0.60400

H 1.0 -2.45073 7.22078 -0.15546  
H 1.0 -2.59513 6.95120 1.58205  
H 1.0 -6.75654 3.82813 -0.06998  
H 1.0 -7.50641 1.49686 -0.45358  
H 1.0 -2.66383 2.51219 -0.03383  
H 1.0 -3.41937 0.18693 -0.43205  
N 7.0 -3.17678 -3.97002 1.51258  
N 7.0 -3.33335 -6.20913 1.57460  
B 5.0 -4.21822 -5.02689 1.42146  
B 5.0 -2.30243 -5.16261 1.35408  
B 5.0 -3.15768 -3.15806 0.32997  
B 5.0 -3.43605 -7.08280 0.43449  
N 7.0 -5.41008 -4.96524 0.61714  
N 7.0 -1.17252 -5.26656 0.46899  
N 7.0 -2.06971 -3.10717 -0.67543  
B 5.0 -1.30202 -4.32825 -0.67280  
B 5.0 -1.43766 -6.24172 -0.62229  
N 7.0 -2.36213 -7.34233 -0.55931  
N 7.0 -4.60125 -7.18423 -0.48189  
B 5.0 -5.36203 -5.96400 -0.48466  
B 5.0 -5.23264 -4.05157 -0.53492  
N 7.0 -4.30873 -2.93552 -0.59875  
B 5.0 -3.22643 -3.20756 -1.59522  
N 7.0 -1.25504 -5.32209 -1.77535  
B 5.0 -3.50485 -7.13088 -1.48434  
N 7.0 -5.49266 -5.02083 -1.62603  
B 5.0 -4.36296 -5.12604 -2.51164  
N 7.0 -3.48953 -6.31622 -2.67109  
B 5.0 -2.44699 -5.26188 -2.57915  
N 7.0 -3.33266 -4.07726 -2.73180

### **Coordinates of CMP-3**

C 6.0 -4.16413 2.85633 0.08335  
C 6.0 -3.13999 3.81733 0.05555  
C 6.0 -1.81276 3.40815 0.26519  
C 6.0 -1.53600 2.06383 0.50171  
C 6.0 -2.56893 1.13522 0.51185

C 6.0 -3.88949 1.50992 0.30581  
O 8.0 -2.24871 -0.21675 0.76524  
H 1.0 -1.34959 -0.47160 0.50428  
N 7.0 -3.50337 5.15693 -0.18486  
C 6.0 -2.68480 6.26493 -0.29555  
H 1.0 -4.49298 5.31692 -0.30513  
O 8.0 -1.46854 6.22557 -0.18461  
C 6.0 -3.41456 7.57310 -0.56655  
H 1.0 -4.49874 7.47740 -0.67591  
H 1.0 -2.99947 8.01053 -1.47841  
H 1.0 -3.19885 8.26236 0.25459  
H 1.0 -5.19459 3.16070 -0.07973  
H 1.0 -4.67462 0.76559 0.28406  
H 1.0 -1.01856 4.13918 0.24365  
H 1.0 -0.51067 1.74955 0.68255  
N 7.0 -6.20053 -2.81884 1.34940  
N 7.0 -6.12076 -5.06610 1.28753  
B 5.0 -6.16456 -3.91242 0.34848  
B 5.0 -5.84234 -3.95291 2.23638  
B 5.0 -5.05913 -1.94464 1.17598  
B 5.0 -4.93664 -5.85435 1.06818  
N 7.0 -5.52984 -3.84565 -0.94039  
N 7.0 -4.81407 -3.93627 3.24107  
N 7.0 -3.95768 -1.73843 2.12707  
B 5.0 -3.77224 -2.91658 2.90815  
B 5.0 -3.69825 -4.83973 2.86999  
N 7.0 -3.79599 -5.99457 2.01029  
N 7.0 -4.17571 -5.94746 -0.20647  
B 5.0 -4.36081 -4.75704 -0.99974  
B 5.0 -4.42929 -2.83507 -0.92848  
N 7.0 -4.33677 -1.68767 -0.08543  
B 5.0 -3.10532 -1.63915 0.84789  
N 7.0 -2.60287 -3.83720 2.86144  
B 5.0 -3.04623 -5.77213 0.74503  
N 7.0 -3.31753 -3.74688 -1.31230  
B 5.0 -2.29436 -3.73799 -0.29949  
N 7.0 -1.92860 -4.88614 0.57396  
B 5.0 -1.97421 -3.77855 1.56809  
N 7.0 -1.99826 -2.63660 0.63484