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B_{84}: A quasi-planar boron cluster stabilized with hexagonal holes

Amol B. Rahane[†] and Vijay Kumar*[†,‡]
[†]Dr. Vijay Kumar Foundation, 1969, Sector 4, Gurgaon - 122 001, Haryana, India.
[‡]Center for Informatics, School of Natural Sciences, Shiv Nadar University, NH-91, Tehsil Dadri, Gautam Budh Nagar 201314, Uttar Pradesh, India.

E-mail: amol_rahane2000@yahoo.com,amolrahane@vkf.in; kumar@vkf.in,vijay.kumar@snu.edu.in
*Corresponding Author

Supplementary Information

Atomic structure: Figure S1 shows the top view and side view of the quasi-planar isomer of B_{84}. The B-B bond lengths are also shown. The top view shows the four hexagonal holes whereas the side view shows that this cluster is quasi-planar and has a bowl-shape. The atomic positions are given in Table S1.

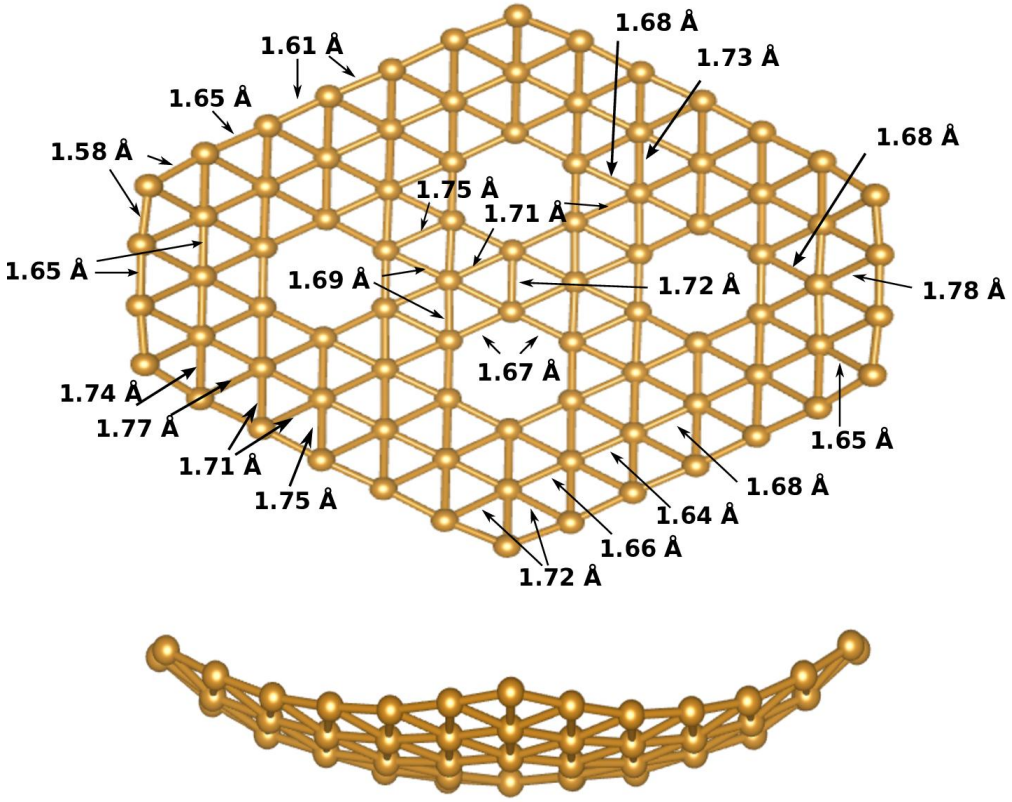

Figure S1: Top view (above) and side view (below) of the lowest energy isomer for B_{84}. The B-B bond lengths are also shown.

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Table S1: Atomic positions for the lowest energy isomer (Figure S1) of B_{84} in Cartesian coordinates (Å).

Atom	x	y	z
B	4.2323401190	3.3248601190	1.0431597619
B	-0.0268198810	5.7604101190	0.2429297619
B	2.7565201190	2.4708301190	1.3069597619
B	-0.1096598810	4.1290701190	0.7885197619
B	-2.9097398810	4.1648401190	0.0695797619
B	2.7801901190	0.7599501190	1.3975597619
B	-1.5502398810	3.2868901190	0.6765197619
B	2.7881301190	-2.5630298810	1.0320297619
B	-0.1746598810	0.7941601190	1.1868897619
B	-1.4777998810	4.9580901190	0.2113997619
B	2.7796901190	4.1523901190	0.8934797619
B	4.2052001190	1.6271901190	1.3513797619
B	2.7904501190	-0.8720998810	1.3088997619
B	-0.0569798810	-4.1906998810	0.3337797619
B	1.3702701190	4.9520301190	0.6224197619
B	-3.0568798810	-0.8629398810	0.4581897619
B	-3.0108598810	2.4813001190	0.4648797619
B	-1.5617598810	-1.7436598810	0.6936397619
B	4.2262001190	-1.7112698810	1.1694197619
B	-1.5081898810	-3.3597098810	0.3134597619
B	-4.4114098810	1.6420001190	0.0818097619
B	-4.3904198810	-1.6963998810	-0.1000102381
B	-4.3445098810	3.3405701190	-0.2133302381
B	-2.9788698810	-2.5543898810	0.1896997619
B	1.2670101190	1.6331901190	1.2877797619
B	1.3067701190	-0.0605998810	1.2661697619
B	-1.6189898810	-0.0556198810	0.8361397619
B	-1.5831998810	1.6384701190	0.8785197619
B	-0.1637898810	-0.9201698810	1.0929297619
B	-5.6219998810	-2.4783198810	-1.0108502381
B	-5.7469898810	-0.8426898810	-0.5746502381
B	-5.7575098810	0.8278001190	-0.4837302381

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B	-5.5394198810	4.1723601190	-1.1106002381
B	-2.8013898810	5.7719801190	-0.4790102381
B	-1.3698198810	6.5965301190	-0.4486702381
B	5.6551601190	0.8077801190	1.2053697619
B	5.6656901190	-0.8627598810	1.1144497619
B	5.6659701190	-2.4959998810	0.6508097619
B	1.4329501190	-4.9723798810	0.0807397619
B	0.0458401190	-5.7522898810	-0.3849502381
B	-1.4152498810	-4.9698098810	-0.3294902381
B	-2.8571098810	-4.1838098810	-0.3854102381
B	-4.3024798810	-3.3519798810	-0.5775202381
B	2.8323001190	-4.1892798810	0.4382097619
B	4.2744601190	-3.3650098810	0.6789397619
B	-5.6528998810	2.5024601190	-0.7405002381
B	-4.2101298810	5.0099101190	-0.7398102381
B	5.6343801190	2.4814301190	0.9204897619
B	7.0860001190	-1.6321298810	0.5463397619
B	7.0748701190	0.0017601190	0.7853697619
B	7.0652401190	1.6520001190	0.7245297619
B	-6.9429998810	-1.6079098810	-1.5320102381
B	-6.9894898810	0.0272601190	-1.3091502381
B	-6.9634698810	1.6772701190	-1.3535402381
B	-6.8419998810	3.3777501190	-1.7274102381
B	-3.0670898810	0.7697701190	0.5470197619
B	1.2998201190	3.2809901190	1.0871097619
B	1.2882901190	-1.7470298810	1.1031797619
B	1.3417201190	-3.3626798810	0.7241897619
B	1.5441401190	-6.5276698810	-0.7545802381
B	2.9118501190	-5.7266498810	-0.2862102381
B	4.3242301190	-4.9631898810	-0.0455902381
B	5.6910701190	-4.1128498810	0.0807697619
B	7.1054901190	-3.2786598810	-0.0326602381
B	8.3621101190	-2.3329998810	-0.2511502381
B	8.4828101190	0.8726201190	0.1164897619
B	8.4933301190	-0.7738498810	0.0272797619
B	8.3316601190	2.4509301190	0.0079797619
B	7.0633201190	3.3515301190	0.3264097619

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B	5.6387501190	4.1507401190	0.5294197619
B	4.2613401190	4.9927001190	0.4959897619
B	2.8393001190	5.7599801190	0.3397597619
B	1.4614601190	6.5898601190	-0.0396802381
B	0.0812501190	7.2434201190	-0.4792902381
B	0.1717201190	-7.1473798810	-1.2625202381
B	-1.2872598810	-6.5255998810	-1.1632902381
B	-2.7291898810	-5.7207998810	-1.1043702381
B	-4.1476598810	-4.9526798810	-1.2816902381
B	-5.4876498810	-4.0965298810	-1.5601402381
B	-6.8007998810	-3.2562698810	-2.0875402381
B	-7.9313898810	-2.3049898810	-2.6689302381
B	-8.1296998810	-0.7440298810	-2.4452902381
B	-8.1398898810	0.9026901190	-2.3560602381
B	-7.9609298810	2.4810501190	-2.4093502381

IR and Raman spectra: The displacement vectors for the dominant IR and Raman active modes are shown in Figure S2. For the IR spectrum there are three dominant peaks at the frequencies 766.89 cm^{-1}, 992.32 cm^{-1}, and 1026.43 cm^{-1}. These IR modes are the combination of the stretching and bending vibrations. For the Raman spectra there are three dominant peaks at the frequencies 1153.09 cm^{-1}, 1222.20 cm^{-1}, and 1350.43 cm^{-1}. The Raman modes are combinations of stretching, bending as well as breathing vibrations. The highest frequency mode at 1350.43 cm^{-1} corresponds to stretching vibrations of the atoms at the peripheral chain. Note that the bond distances for these atoms are the shortest.

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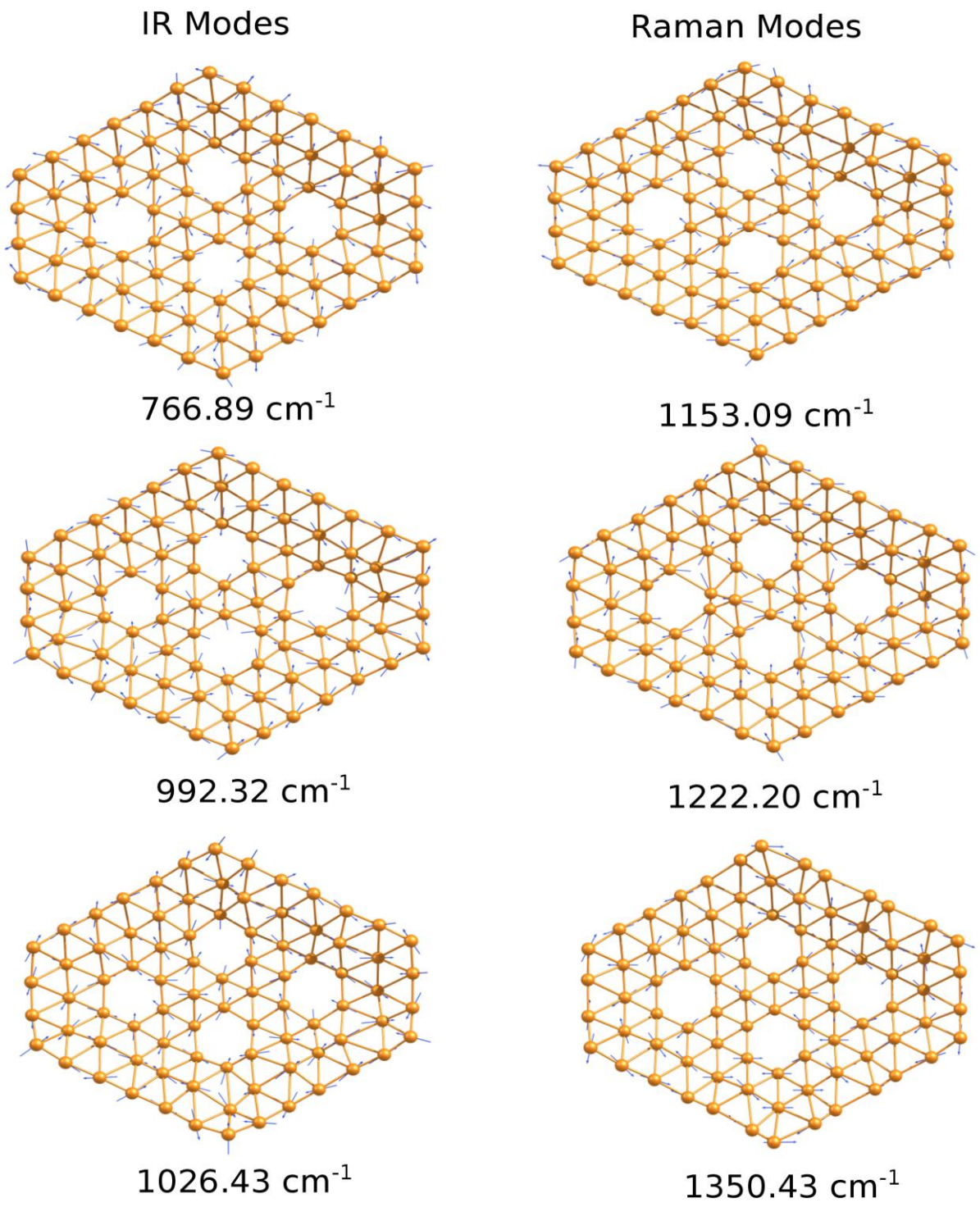

Figure S2: Displacement vectors are shown by arrows for the dominant IR (Left Side) and Raman (Right Side) active modes for the lowest energy isomer of B_{84}. The corresponding frequencies are also given.

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Charge Transfer Analysis: We have calculated the charge around each atom using the Voronoi partitioning as implemented in the Bader program. The Voronoi analysis (Figure S3) shows that atoms on the peripheral chain and on the edges of the hexagonal holes have excess charge, whereas depletion of charge can be seen on the atoms which are surrounded with six neighbours.

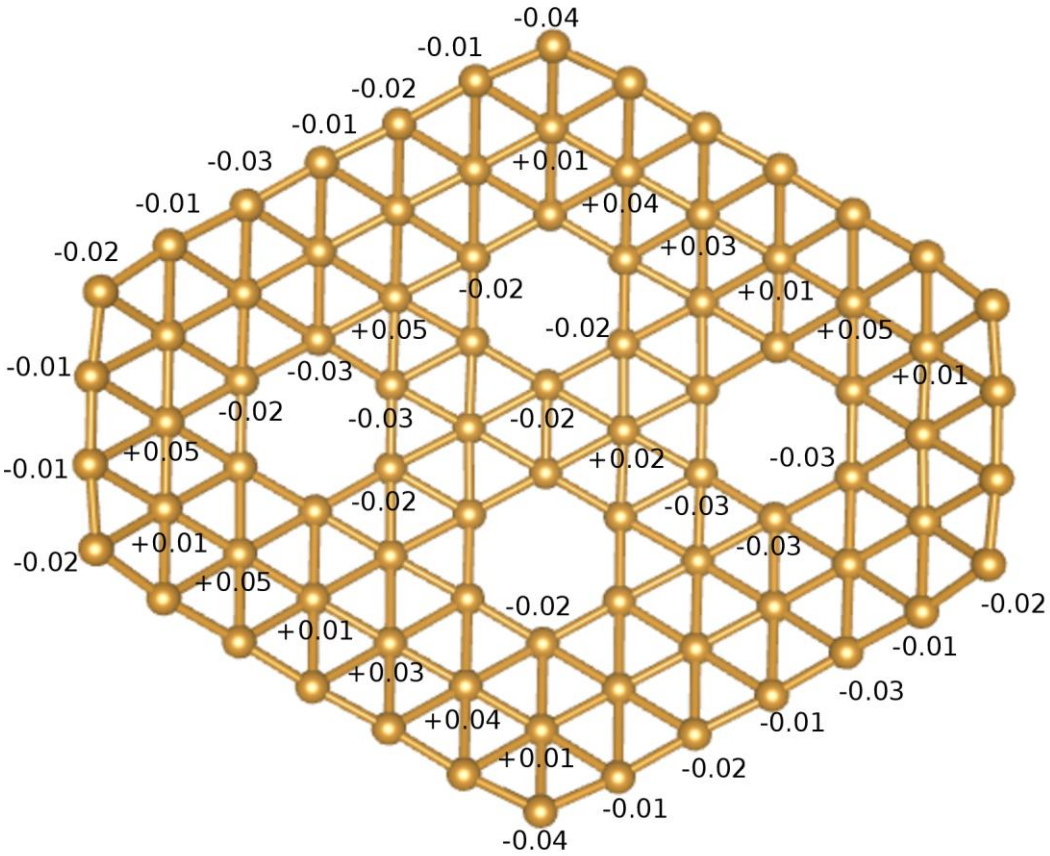

Figure S3: Calculated charge transfer using Voronoi partitioning for the lowest energy isomer of B_{84}. The charges are calculated using the Bader program [Ref. W. Tang, E. Sanville and G. Henkelman *J. Phys.: Condens. Matter.* **21**, 084204 (2009)].