Bucky's brother -- The boron buckyball makes its debut

April 23 2007

A new study by Rice University scientists predicts the existence and stability of another "buckyball" consisting entirely of boron atoms.

The research, which has been published online and is due to appear as an editor's selection in *Physical Review Letters*, was conducted bv Boris Yakobson, professor of mechanical engineering and materials science and of chemistry, and his associates Nevill Gonzalez Szwacki and Arta Sadrzadeh.

The original buckyball, a cage-shaped molecule of 60 carbon atoms, was discovered at Rice by Robert Curl, Harold Kroto and Richard Smalley in 1985. The boron buckyball is structurally similar to the original C60 fullerene, but it has an additional atom in the center of each hexagon, which significantly increases stability.

"This is the first prediction of its possible existence," Yakobson said of the boron buckyball, or B80. "This has not been observed or even conceived of before. We do hope it may lead to a significant breakthrough."

In the earliest stages of their work, the team attempted to build a "buckyball" using silicon atoms but determined that it would collapse on itself. Their search for another possible atom led them on a short trip across the periodic table.

"Boron is nearby (one atomic unit from carbon). One reason we tried it

was because of proximity," Yakobson said. "Boron also has the ability to catenate, to stick together better, than other atoms, which also made it appealing."

Initial work with 60 boron atoms failed to create a hollow ball that would hold its form, so another boron atom was placed into the center of each hexagon for added stability.

Yakobson estimated that the scientific work, the consideration of the variety of boron clusters to single out the B80, took more than a year, with Szwacki initially leading the work and then Sadrzadeh gradually taking greater part in the effort.

"We thought we had the answer, essentially, after three or four months, but then we had to prove it," Yakobson said. "There are numerous possibilities, but we had to prove that this was the answer. I think we've made a convincing case."

Yakobson said it is too early to speculate whether the boron buckyball will prove to be equally or more useful than its Nobel Prize-winning sibling.

"It's too early to make comparisons," he said. "All we know is that it's a very logical, very stable structure likely to exist.

"But this opens up a whole new direction, a whole new continent to explore. There should be a strong effort to find it experimentally. That may not be an easy path, but we gave them a good road map."

Following the paper's acceptance, there was a little debate with the journal's editors about whether or not the structure could be named "buckyball." Yakobson mentioned this to Curl.

"Bob (Curl) said with a chuckle that it was more of a 'buckyball' than his buckyball," Yakobson said. The reason being that C60 was named for famed architect Buckminster Fuller, because the buckyball looked like conjoined geodesic domes, a structure that Fuller had invented.

"When Fuller made his domes, he made them from triangles because hexagons would collapse," Yakobson said. "In B80, we fill the hexagon with one more atom, making triangles."

Yakobson said having the paper published in *Physical Review Letters* will help get the attention of experimentalists in the field.

"It is very helpful that this work can be seen and this is just a good instrument for it," he said. "To be able to deliver it to this broad a base of physicists and chemists is a good start."

Source: Rice University