Catching buckyballs

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Buckycatchers

Buckminster Fullerene is one of the most iconic molecules that chemistry has to offer. Maybe it is the high symmetry or the fact that it consists exclusively of carbon atoms, but C60 has captured the imagination of many researchers since its discovery almost thirty years ago.

So far, no commercial applications that use fullerenes have been successfully marketed. This is partly due to the fact that it is difficult to manipulate individual C60 molecules to make the necessary changes for each application. In our work, we discuss the possibility of “catch and release” complexes where we use functionalised Buckybowls, large carbon-rich molecules that are derived from corannulene and have a curvature that is very similar to that of fullerene, to reversibly bind to C60.

Because the fullerene and the corannulene molecules bind through very weak van-der-Waals type forces that are computationally difficult to describe, a careful benchmarking of available theoretical methods was employed to ascertain the best physical representation of the real system at the lowest possible computational cost. Armed with the results of this extensive study, we then proceeded compute a large array of Buckyball-Buckycatcher complexes. Because the structural information that is so readily available to theoretical chemists is difficult to compare to routinely obtained experimental results, we also calculated predicted NMR spectra for the complexes in our study. When the spectroscopic results were analysed, we discovered that intriguing correlations sometimes exist between the binding strength of the host-guest molecular complex and some of the observed NMR signals. This will serve as a valuable tool for experimentalists trying to ascertain which changes in their proposed Buckycatchers’ structure will improve its ability to “catch” a Buckyball.

Figure: A Buckycatcher-Buckyball complex.
Computational chemistry on the Pan cluster

Modelling chemistry on the computer is a classic application of High Performance Supercomputers, and has been ever since the very early days of HPC facilities. Our research follows in that tradition and employs large scale parallel calculations that use large amounts of both memory and CPU-core time. The throughput of computational clusters is especially important to us, because it allows the pointwise construction of potential energy surfaces. In addition to this memory and CPU time, more complex computations, like the prediction of NMR chemical shifts and coupling constants, can also require large amounts of disk space to store intermediate data. A well balanced computational cluster that offers all three of these resources in combination with a fast network connection across New Zealand is essential to obtaining our results.

What next?

The next step for us will be to extend this investigation into the redox chemistry of the Buckybowls, in order to optimise the release of the Buckyball from its Buckycatcher. This significantly different problem involves changes in the electronic structure of the corannulene derivatives, and hence the complexes, and will require an entirely new set of calculations.

Contact details

This work “Accurate Density Functional Theory Description of Binding Constants and NMR Chemical Shifts of Weakly Interacting Complexes of C60 with Corannulene-Based Molecular Bowls” is published online in the Journal of Computational Chemistry, currently as early view), DOI: 10.1002/jcc.23455 where it will be featured on an upcoming journal cover.
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