WHERE CAN I FIND A COMPUTATIONAL CHEMIST?

In the United States, we have developed a phenomenon called the 'headhunter'. For those of you who are not familiar with this nomenclature, the headhunter serves a rather important role, and is only brought into action when there is a problem.

A headhunter is a personnel consultant who is paid rather significant sums of money to find a very special type of employee for some corporation. Often these personnel searches are for Chief Executive Officers, Chief Financial Officers, etc. Headhunters receive fees like $15000, and sometimes much more, for finding the critical person in question.

Recently, QCPE has been receiving furtive phone calls from such people who are desperately seeking something called a 'computational chemist'. The headhunter is not quite certain what one of these looks like, and often a great portion of the communication process is given over to coming up with a proper description of these creatures. There appears to be no real consensus as to what one of these entities even does. The definition varies with the company. What is even more troublesome for the personnel consultant is the vocabulary which is used in describing a properly dressed computational chemist. There are words like MOPAC, Molecular Mechanics, Ab Initio, wavefunction, etc. However, a good headhunter is always willing to upgrade his level of knowledge if he can find someone who will work with him; besides, he will be paid handsomely if he can capture one of these creatures. The bounty for bringing in one of these is noteworthy and it goes without saying that they must be alive.

I am certain that, by this point, many of you are saying that there are many ads to be found in trade publications relating to computational chemists. One simply prepares a résumé and sends it to the personnel department and they sort through all the entrants for the competition and ultimately announce a winner. Things, unfortunately, just aren't that simple.

What happened when a few corporations tried this approach was a bit surprising. They discovered that there were suddenly hundreds of computational chemists available. Every chemist who happened to be looking for a new job and who had had any contact whatsoever with computational chemistry had reworked his or her résumé, and was now applying for the job. When the personnel people tried to sort through this vast response they came to the alarming conclusion that, in reality, none of them knew what a computational chemist should look like. It was at this point that the task was thrown to the professional personnel consultant (headhunter).

In other corporations which have yet to confront this problem, the personnel function goes about its business in smug comfort. In one situation which has come to my attention, a recent graduate with an extensive background in computational chemistry sent forth a large number of résumés. He received many prompt answers from the personnel departments of these companies, informing him that there was no need for a computational chemist. In the case of at least one of these companies this same applicant received a solicitation from a headhunter on behalf of the company. What the personnel department had turned down they were now about to pay a premium to obtain.

I questioned a professional personnel man of many years experience about how this could happen. His response was that no one in the personnel department understood the résumé. They simply hadn't related what the research division was asking for with what was contained in the résumé. This appears to be a common failing of the personnel function when a new discipline emerges.

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They do not have keywords which they can depend on to sort out the real from the other. Situations like these provide job security for personnel consultants.

The message in all of this is twofold. One, major corporations now place some value on the services of computational chemists. Secondly – and most importantly – it appears that computational chemists are in short supply. The demand for the services of those people who actually can carry the mantle of computational chemist now exceeds the supply. The question as to where one can find a computational chemist is a very real one.

The core problem is that there is no systematic way in which computational chemists are produced. One cannot look to universities to produce them. It is true that, on occasion, one will emerge from a university, but that is more happenstance than anything else. The reason is very simple. Universities are organized along disciplinary lines. Chemistry departments produce organic, inorganic, physical, etc., chemists. The computational chemist is more focused on problem-solving than upon a single field of chemistry. In fact, one must be willing to work accross all the traditional fields of chemistry to be an effective computational chemist. So we are brought back to the original question: Where can I find a computational chemist?

There now appears to be something approximating a consensus emerging among people who worry about such things. The current wisdom is that industry must begin to consider training its own people. As a starting point, an organic chemist with an interest in computational approach seems to produce the best results.

What one gets is a person to whom chemistry and the changes which it produces in physical properties as well as chemical properties is very real; it is not an abstraction of the mathematical variety. This viewpoint, when combined with the computational tools now available, tends to produce some extremely innovative solutions to product problems. One of the more inspirational solutions to a product problem which I can recall came from just such a person at an IBM laboratory.

The problem which was so elegantly solved using computational chemistry related to perfluoro lubricants which are used to protect the surfaces of computer disk drives. It was found that there was a deleterious catalytic interaction taking place between the lubricant in use and the metal oxide surface material of the disk. The lubricant in question had all the desired physical properties. What was needed was this lubricant but with different chemical properties.

The researcher discovered that this same lubricant in a branched structure, as opposed to the unbranched structure currently in use, had all the correct physical properties but its chemical properties with regard to the destructive chemical interaction had now changed. This latter information about the chemistry involved came from looking at the difference in wave functions between the two versions of the lubricant molecule.

It may not be possible to produce this type of person in a systematic way. They may have to be simply looked upon as some form of artisan. We are fairly certain, however, that starting with a chemist and adding on the additional skills is the surest way of producing something productive fairly quickly. Possibly, after we have produced enough of these people and abstracted from this experience what it takes to lay the foundation for producing such chemists, we will one day be able to meet the demand which we are experiencing. Until that time, however, we may be reduced to hiring way each other's employees.

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