CALIFORNIA STATE SCIENCE FAIR
2003 PROJECT SUMMARY

Name(s)
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Project Number
S1516

Project Title
Computer Simulation of van der Waals Clusters

Abstract

Objectives/Goals
Van der Waals clusters are groups of chemically neutral atoms or molecules with weak forces of attraction, the Van der Waals forces. They occur naturally and are created in laboratories by jet expansion. My objectives were to study the properties of Van der Waals clusters by computer simulation. I was interested in finding if and how the structures and stabilities of the clusters depend on their sizes.

Methods/Materials
I wrote two computer programs (for two-dimensional and three-dimensional clusters) in C to model the configurations of clusters of different sizes. I used the Monte Carlo method in my algorithm to find the equilibrium configurations. I plotted the configurations of the clusters and I compared their stabilities and analyzed their properties.

Results
I found that all the two-dimensional clusters are sections of a hexagonal lattice. All the clusters are very compact and symmetrical. The most stable two-dimensional clusters are the most symmetrical. Thus the most stable three-dimensional clusters must also be the most symmetrical.

Conclusions/Discussion
This information can help me analyze and interpret results for larger clusters that cannot be pictured. Finally, a parallel can be drawn between clusters and atoms. Just as atoms have certain sizes that make them most stable, namely the inert gases, so do clusters.

Summary Statement
I studied the properties of Van der Waals clusters by computer simulation.

Help Received
My father helped run my programs on his computers and gave me general advice on numerical algorithms; my mother helped proofread my report; a friend helped fix syntax errors in my program.