THE IRREDUCIBLE BUNDLE: ITS METHOD, CONTENT, AND MEANING

by

Travis E. Jones

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Golden, Colorado

Date 3/2/11

Signed: ______________________

Travis E. Jones

Approved: ______________________

Dr. Mark E. Eberhart
Professor of Chemistry
Thesis Advisor

Golden, Colorado

Date 3/2/11

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Dr. Daniel M. Knauss
Professor and Head
Department of Chemistry and Geochemistry

ABSTRACT

The chemical formalism developed over the last 100 years provides the capability to design molecules and solids with desired properties. However, there are classes of materials to which this formalism is not applicable, the fracture of metals and alloys, for example. It is the absence of well defined "bonds" in these materials that confounds the analysis of such phenomena from a chemical perspective. Here, a topological model of molecular structure is developed. When mature it will allow the formalism of chemistry to be brought to bear on problems not typically considered chemical in nature. While it will take time to fully develop the underlying concepts and methods, the work presented here lays the foundation.

This thesis is broken into four parts i) Chapter 2 develops the concept of a topological bond. ii) Chapter 3 shows that far from being a convenient construct, the surfaces of topological bonds are physically meaningful. iii) The physical significance of these bonds is further developed in Chapter 4, where it is shown that the volume of a topological bond serves as an order parameter of a continuos phase transition. iv) After showing that the topological bonds are not merely constructs, Chapter 5 goes on to show how these bonds can be used to solve nontraditional problems of chemistry, such as fracture of an iron/ceramic interface.

The model is an extension of Bader's Atoms in Molecules (AIM) theory. AIM theory posits that volumes bound by surfaces of zero flux in the gradient of the electron charge density have well-defined and additive properties. Thus, it becomes possible to partition space into subsystems characterized by measurable and calculable properties. The advantages of this approach are clear. Unlike other theories of