UNUSUAL OXIDATION STATES AND COORDINATION NUMBERS OF THE LIGHT ELEMENTS.

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The research under this contract was devoted to the development and testing of quantum mechanical techniques suitable for studying novel geometries, coordination and oxidation states of the light elements. Prediction of stabilities and various aspects of their chemistry was also made for numerous molecular complexes of these elements. In particular, HeF\(^+\), NeF\(^+\), HeO\(^+\), NeO\(^+\), HeN\(^+\), NeN\(^+\), ArO\(^+\), and ArF\(^+\), generally in combination with the counter ions PtF\(_6\)^\(\rm-\) and SbF\(_6\)^\(\rm-\), are expected to show stability in one or several molecular states. The existence of noble gas boron compounds also appears possible under appropriate circumstances.

Three graduate students and one postdoctoral research associate were trained under this contract and two of these have continued in this general area and are themselves currently producing important new chemical information that is certain to aid the mission of ONR.

It is possible to make a general conclusion from the specific research funded by this contract that should be of far reaching significance to ONR. Even though none of the particular compounds studied have ended up in fleet usage, a new theoretical capability was demonstrated which is in many ways on an equal footing with traditional experimental techniques and which in some cases may have a decided economic advantage. This new theoretical approach is currently being employed in numerous laboratories and is largely the result of continued advances in applied quantum mechanics and in the revolutionary changes in computer hardware and software. The method is basically "numerical experiments" and as such it is well matched to the subject matter of chemistry and to traditional "instrumental experiments".

Scientific and technical details of the research supported by this contract and acknowledged to it have been reported in the following scientific journal articles:


Unusual Oxidation States and Coordination Numbers of the Light Elements

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Office of Naval Research (CODE 473)
Arlington, Virginia 22217

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Noble gas molecular ions
Electronic structure calculations

Stable states and molecular complexes of HeF^+, HeO^+, HeN^+, NeF^+, NeO^+, NeN^+, ArF^+, and ArO^+ were studied by electronic structure theory calculations. The possible existence of noble gas boron complexes was also investigated.