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Jennifer L. Keedy
Amherst College, Miami, Florida

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IS DIAMAGNETIC OXYGEN PRESENT IN SPACE?
(GETAWAY SPECIAL PROGRAM)

JENNIFER L. KEEDY
AMHERST COLLEGE
POST OFFICE BOX 687
AMHERST, MA 01002
5257 SW 92 STREET
MIAMI, FLORIDA 33156

ABSTRACT
The formation of the oxygen dication, \( \text{O}_2^{2+} \), is predicted to occur in significant quantities in the earth's upper atmosphere and in space. This species is diamagnetic and has been detected in various experiments on earth. It is very reactive. Cosmic rays may provide the energy needed to form the dication from the uncharged molecule. The vacuous environment of space could insure a measurable lifetime for the ion. Properties and uses of diamagnetic oxygen are discussed.

INTRODUCTION
According to the Bohr theory of atomic structure, an atom consists of three basic kinds of particles: electrons, protons, and neutrons. An electron is a particle which has a negative charge, and a proton has a positive electric charge of equal magnitude to an electron. A neutron has no charge. Surrounding the nucleus, which contains the neutrons and protons, are shells of electrons carrying sufficient negative charge to offset the nuclear positive charge. Thus, an uncharged atom has equal numbers of electrons and protons. The Bohr model is analogous to the planets revolving about the sun in our solar system (see figure 1).

Quantum theory describes the distribution of electrons in an atom in more detail, placing them in subshells, or orbitals. An orbital is a region of space surrounding the nucleus where electrons are most likely to be found. Molecular orbital theory extends quantum mechanics and describes the probability of finding electrons within certain regions of molecules. Molecular orbitals are postulated to surround the various nuclei present in a molecule. The electrons within these orbitals are envisioned as constantly moving about over the entire molecule.

The molecular orbitals in a diatomic molecule result from a combination of two sets of atomic orbitals. One kind of molecular orbital results from the addition of parts of the orbitals which overlap and is known as a bonding orbital. The other kind of molecular orbital results from the subtraction of the overlapping parts of the atomic orbitals and is known as an anti-bonding orbital. Of the two kinds of molecular orbitals, the bonding orbital is of lower energy than the antibonding orbital, and therefore, the molecule's electrons tend to fill the bonding orbital's in preference to the antibonding orbitals. At most, two electrons may occupy any given orbital.

An electron rotates about its own axis in either a clockwise or a counter-clockwise direction; this is referred to as the electron's spin. According to Hund's rule, the electrons in a molecule enter the available orbitals of a given energy individually and with identical spins before any pairing of electrons with opposite spins occurs within the orbitals. The fully occupied orbital therefore has two electrons, each with a different spin.

The diatomic oxygen molecule (\( \text{O}_2 \)) is paramagnetic; this means it is attracted by a magnetic field and orients itself parallel to the magnetic lines of force. Paramagnetism arises because a molecule contains one or more unpaired electrons. Therefore, it has a net spin which gives rise to magnetic properties. Diatomic oxygen has two unpaired electrons in its molecular orbital structure (see figure 2). If the "correct" energy (i.e., that defined by quantum mechanics) is added to the oxygen molecule, the electrons will pair; this gives rise to a species known as singlet oxygen. The energy goes into reversing the spin of one of the electrons, and then all electrons are
paired; the singlet oxygen is no longer paramagnetic. If additional energy is added, ionization occurs yielding oxygen cation, $O_2^+$, and an electron. More recently, at the Georgia Institute of Technology the oxygen cation has been further ionized to form the dication.

**PROPOSAL**

I hypothesize that the oxygen dication, $O_2^{2+}$, should form in the earth's upper atmosphere and in space. There should be enough energy from cosmic radiation to produce it, and because of the low concentration of molecules in these regions, the ion should be stable. The oxygen dication might be generated by collision of the neutral or singly charged oxygen species with electrons (beta rays), or cosmic, gamma, or ultraviolet radiation. These types of radiation are energetic enough to effect the pi* to sigma* transitions required in the initial stages of ionization (see above and figure 2). In other words, the highest energy electron in both the neutral and monocationic species is found in the pi* (antibonding) orbital, and will absorb energy and jump to the next orbital, sigma*. Additional energy will cause the electron to be lost, thus generating an ion with one more positive charge. Work at the Georgia Institute of Technology has verified the expectation that the molecular structure of the oxygen dication is similar to that of diatomic nitrogen, which has no unpaired electrons and a triple bond between the two atoms (see figure 3).

Because the oxygen dication has no unpaired electrons, it is diamagnetic. This means that it will not respond to a magnetic field. To detect the presence of diamagnetic oxygen in the upper atmosphere, a sample must be taken and analyzed for the ion. The analyzer must be able to house the ion (in an electromagnetic field) and be able to detect trace amounts of it, since it is a very reactive species in the presence of other molecules. I suggest a trace method such as that afforded by the electrostatic-magnetic apparatus used in the detection of the laboratory-generated ion at Georgia Tech. Their detector uses an electrostatic field to determine the energy of a species and a magnetic field to determine its momentum. Such a device will separate the double charged oxygen from the monocation and all other molecules in the system. The dication and monocation have mass to charge ratios of sixteen and thirty-two, respectively, and are separated on this basis. A similar method, using mass spectroscopy, was employed successfully in detecting trace amounts of gases in Skylab experiments.

If the oxygen dication is shown to be present in the upper atmosphere, it could be very useful. It should be a highly effective oxidizing agent which, unlike uncharged molecular oxygen, is electrophilic. It should therefore react with electron rich compounds such as benzene in ways that are completely unknown. Moreover, it could speed up slow oxidation processes including the decay of organic matter and the transformation of carbon monoxide to carbon dioxide. Perhaps it could also be used to form a protective oxide coating on metals so that they do not further oxidize:

$$
Zn^0 + O_2^{2+} \rightarrow (Zn^{2+} + O^0) \rightarrow ZnO^{2+} + ZnO
$$

Another area of exploration would be in analyzing oxygen dication formation in low pressure direct current-discharge plasmas. Such plasmas are useful in polymer surface treatments, etching, chemical synthesis, and polymerization. In addition, the oxygen dication may be used to determine elemental composition, particularly in halogen containing compounds.

**CONCLUSIONS**

Investigations of ionic molecules in space have been extremely limited, and yet ions are very important in many systems, including aurorae, comets, and novas. Not only is the identification of the oxygen dication of academic interest, but it may be of commercial use if found in suitable concentrations in our upper atmosphere. Finally, the dication could be useful in locating solar systems with oxygen "containing" planets. Such experiments must await further characterization of the diamagnetic species. I believe that the upper atmosphere will provide a likely source for such ions.

**ACKNOWLEDGMENTS**

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Figure 1: The Atom as Envisioned by Niels Bohr. Bohr pictured the atom as having a nucleus housing the protons and neutrons about which the electrons rotate.

Figure 2 (above): The Molecular Orbital Representation of Oxygen, \( O_2 \). Note the unpaired electrons of highest energy in the \( \pi^* \) (antibonding) orbital.

Figure 3 (right): The Lewis Structure of Oxygen is shown with normal double bond (top). Absorption of energy by electrons results in the transformation shown in the middle diagram. If two electrons are lost, the bottom structure, with a triple bond, is formed.