IS Q FOR QUANTUM? FROM QUANTUM MECHANICS TO FORMATION OF THE SOLAR SYSTEM.

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Introduction: The realization in 1985 that fullerenes exist in nature [1] as a third form of carbon-carbon clustering, continues to inspire new areas of research. In particular, the study of closed-cage endohedral fullerenes [2-6] is of scientific interest because of its potential application in a number of promising fields from medical imaging to astrophysics. One of these is to provide a possible chronometer for studying the age and origin of certain astromaterials in the solar system. Fullerenes are closed carbon cages that are fundamentally related to a long-standing debate over the "Q-Phase" origin of planetary noble gases in carbonaceous chondrites [7]. Although Q-phase has been identified as the carrier of planetary noble gases [8-10], its physical nature has not been explained. Our limited understanding of it is based primarily on the laboratory chemical processing which it survives as well as the fact that it must have been widely distributed in the solar nebula [11]. Yet as important as it might be while preoccupying some 30 years of research, the question of what actually is Q-phase remains unresolved.

Are carbon cages Q-phase?: As depicted in Figure 1, the internal cavities of fullerene objects are large enough (up to ~7 Å in radius) to encapsulate complete atoms [1-5] and even molecules, forming endohedral configurations ranging from He@C_{60} to Xe@C_{60}. Such cages can be produced when fullerenes are formed under pressure in the presence of a noble gas. Conjectures were eventually made that Q-phase may be fullerenes [12] or carbon nanotubes [13]. These investigations remain negative or inconclusive [14-17].

One reason for much of the caution has been the realization that carbon graphite clusters can morph into complicated geometries and symmetries. In the laboratory using energetic electron beams, onion-type configurations of fullerenes within fullerenes have been created [18, 19]. Subsequently it was shown that these carbon onions can be easily and readily produced [20] by running a charged current between carbon cathodes in ordinary water. Lightning on Earth [21] or a relativistic plasma in space might accomplish a similar thing.

Regardless of the ultimate answer, the stability of carbon clusters is a complex subject involving chemical dynamics [22-23], quantum chemistry [24-25], and quantum mechanics. Since fullerene has been found to be a quantum object [26], quantum mechanics has now become a part of cosmochemistry.

Basic quantum issue – nothing lives forever: Quantum physics changed science in a number of ways, one of which was to demonstrate that many states of matter are unstable and decay. The endohedral noble gas entrapped in Figure 1 will tunnel through the carbon cage without it being opened by some chemical means. Whatever quantum object can get in there *will* come out of there. Hence, all endohedral carbon cages have finite life-times due to quantum tunnelling.

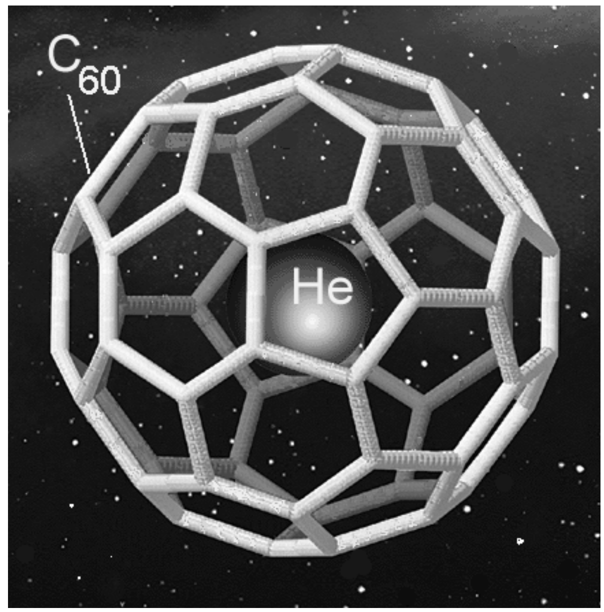

Figure 1. Endohedral fullerenes containing trapped noble gases may represent a type of Q-phase chronometer for investigating their age and origin using quantum mechanics. Carbon atoms are not depicted.

A metaphor is α–decay. As the object shown in Figure 1 approaches a nearby star or an early active Sun, energetic photons can ionize the entrapped He if they penetrate the carbon cage. The He molecule then literally becomes an α-particle in a superpotential of van der Waals and other forces. The configuration is ostensibly a subject of textbook α–decay, and the endohedral cage emits an α-particle. However, be cautious as quantum physics is not always so simple.

Modelling in Quantum Chemistry: Fullerene chemistry has been adapting theoretical models for clathrate cages for some time. The structures and non-bonded intermolecular interactions of endohedral fullerene-noble-gas clusters have been addressed using the atom-atom Lennard-Jones potential method [24-25]. This potential is fundamental to quantum chemistry, mimicking the attracting van der Waals interaction at long distances while using an empirical repulsion (due to overlapping electron orbits) at short distances. It is illustrated in Figure 2 for the Q-phase gases.

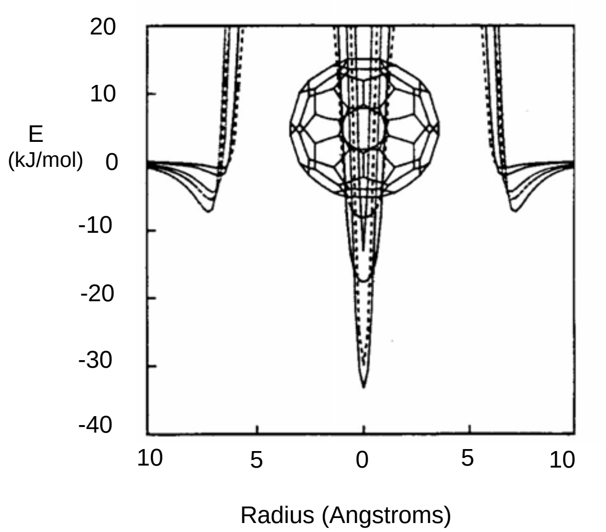

Figure 2. Translational energy E in the Lennard-Jones model for $Q@C_{60}$ clusters (Q = long dash, He; solid, Ne; dotted, Ar; dash, Kr; and dot-dash-dot, Xe). Adapted from [24].

Q-phase tunnelling calculations necessarily require definition of such a quantum potential well [e.g. 27, 28]. The α–decay problem mentioned previously, for example, is an inverse function of the expulsion velocity of the α-particle. Many subjective assumptions can become involved, depending upon the nature of the Q-phase host. Although the ultimate answers for endohedral carbon-cage life-times may be large, the subject is pertinent to understanding planetary physics and cosmochemistry over the age of the solar system. To assume that carbon-cage lifetimes are infinite as has been done heretofore is no longer justified.

Thermal and energetic shock instabilities: Any mechanism that opens the fullerene cage permits the caged guest to escape, found early-on at increased temperature and pressure [3]. Energetic shock effects of bolide impact on Q-phase gas retention and recovery have likewise been conducted at 30, 47, and 70 GPa [29]. The latter pressure showed Q-phase gas expulsion effects. However, the notion that high temperature will destroy the carbon cage is naive, when in fact energetic interactions can cause the single-walled cage to form multiple walls instead, as onions [30, 31] for example. New studies also show that carbon cages can survive high temperatures for short periods of time [32].

Conclusions: The Q-phase carrier of entrapped planetary noble gases has not been identified. Endohedral carbon cages are viable candidates, and these may provide chronometric data about the presolar nebula. We know that planetary noble gases are characterized in part by depletions in light gases relative to heavy gases as compared to the Sun. Quantum effects on carbon cages may offer an explanation of this.

Because fullerene was recently shown to be a quantum object [26], quantum effects have now become relevant to an ultimate understanding of Q-phase. Without these additonal analytical tools, cosmochemistry is incomplete.

Acknowledgements: The authors are grateful for helpful comments from Dr. Don Bogard on this topic.

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