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A unified theory of atomic and nuclear shell structure

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Summary. By stipulating that like-fermions adjacent in space must be singlet paired, geometric considerations alone produce closed electron shells at the 6 noble gases and, similarly, closed nucleon shells and subshells isomorphic with those of the harmonic oscillator used in nuclear theory.

The differences between nuclear and atomic (electron) structure are considerable, due to the inherent differences in scale and constituent particles of the 2 realms. Nevertheless there are some fundamental similarities between them: they are both comprised of fermions and are both known to arrange themselves into symmetrical shells of relative stability and 'inertness'. While of course the quantum mechanical basis of both electrons and nucleons is well known, neither the reason for the specific empirically found shell structures nor the fundamental relationship between them is particularly clear. The build-up of electron shells based upon the empirical findings of the hydrogen atom proceeds: $1s^2$; $2s^2$, $2p^6$; $3s^2$, $3p^6$, $3d^{10}$; $4s^2$, $4p^6$, $4d^{10}$, $4f^{14}$; $5s^2$, $5p^6$, $5d^{10}$, $5f^{14}$, etc. (a comma signifying the closing of a subshell, a semicolon signifying the closing of a shell). Such a build-up process gives theoretical electron shells and subshells at: 2; 4, 10; 12, 18, 28; 30, 36, 46, 60; 62, 68, 78, 92, etc. electrons - among which 4 of the 6 known noble gases appear, but only 2 of them are predicted as closed shells (2 and 10), rather than as subshells (18 and 36). Only by utilizing an empirically based mixing and spacing of these subshells can all 6 noble gases be rationalized. A mixed and appropriately spaced sequence: $1s^2$; $2s^2$, $2p^6$; $3s^2$, $3p^6$; $3d^{10}$, $4s^2$, $4p^6$; $4d^{10}$, $5s^2$, $5p^6$; $4f^{14}$, $5d^{10}$, $6s^2$, $6p^6$; etc. produces shells and subshells at: 2; 4, 10; 12, 18; 28, 30, 36; 46, 48, 54; 68, 78, 80, 86; etc. electrons. The situation in nuclear theory is much the same. The order of build-up according to the isotropic harmonic oscillator potential - which is the basis for the shell model - predicts (depending upon the various possible assumptions concerning the precise nature of the potential well) closed shells and subshells at: 2; 6, 8; 14, 18, 20; 28, 34, 38, 40; 50, 58, 64, 68, 70; 82, 92, 100, 106, 110, 112; 126, etc. protons or neutrons - among which all of the empirically known closed shell numbers appear, but only the 1st 3 (2, 8 and 20) are predicted to be closed shells rather than subshells. Again, an empirically based mixing and spacing of the nuclear subshells is used to rationalize the existence of relatively stable nuclear shells at 2, 8, 20, 50, 82, and 126 protons or neutrons.

In an effort to understand why these particular nuclear and electron shells arise, I have found an unorthodox, yet extremely simple and selfconsistent explanation for both, which is based upon a single principle of fermion interaction. That is, if it is postulated that like-fermions which are adjacent in space must be singlet paired, then the periodicity of both nuclear and electron structure can be rationalized on geometric grounds alone. Such a postulate can be viewed as an expansion of the version of the exclusion principle which states that like-fermions which are 'adjacent' within an energy level must be singlet paired, or, alternatively, it can be seen as a formalization of the concept that in a fermion sea there exists a probability 'hole' for finding a 2nd particle near to a similar 1st particle. The raison d'être for this postulate is presumably that the intrinsic currents of neighboring like-fermions (positive currents in the case of protons and negative currents in the case of electrons and neutrons) give rise to an attractive magnetic interaction when singlet paired, and a repulsive interaction when triplet paired. Since it is questionable whether or not the Biot-Savart law or related macroscopic electromagnetic laws are applicable at a microscopic level and, if not, it is an unanswered question what may be occurring electromagnetically at this level, further energetic questions will not be dealt with here. Instead, a phenomenological correlation between empirical findings and models based upon this postulate will be presented.

Starting with nuclear structure, the singlet pairing of adjacent protons or neutrons implies an antiferromagnetic face centered cubic (FCC) lattice structure with alternating layers of protons and neutrons. This same crystal structure has previously been calculated to be the lowest energy solid configuration of neutrons and protons (N = P) - likely to be found in the interior of neutron stars[1], and has also been shown to rationalize many of the predominant features of normal nuclei[2,3]. Briefly stated, the FCC lattice structure built from a central tetrahedron ($^2_2He^4$) produces closed, symmetrical ($x = y \neq z$) structures at all of the closed shells predicted by the isotropic harmonic oscillator potential,

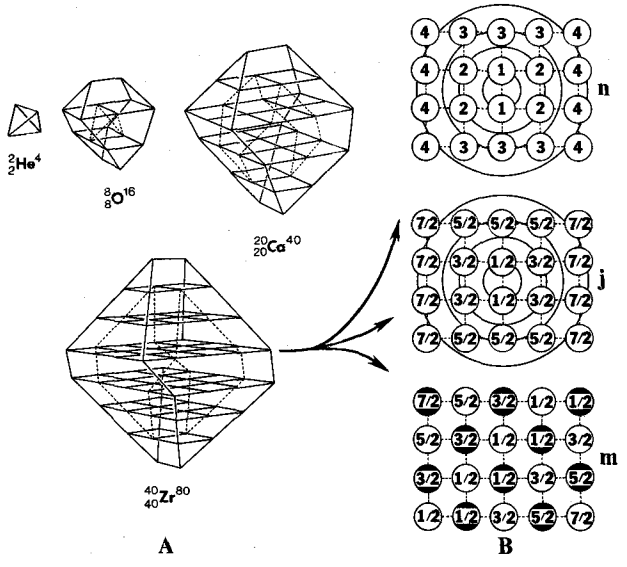

Fig. 1. Nuclear shell structure based upon the antiferromagnetic FCC lattice with alternating layers of protons and neutrons. *A* The shell structure arising from an FCC lattice built from a central tetrahedron produces closed shells at $^{2}_{2}He^{4}$, $^{8}_{8}O^{16}$, $^{20}_{20}Ca^{40}$, $^{40}_{40}Zr^{80}$, $^{70}_{70}Yb^{140}$, and $^{112}_{112}Xx^{224}$. Each shell is shown with the next smaller closed shell drawn inside. Because of the ever-increasing electrostatic repulsion among the protons, N = P nuclei larger than Ca^{40} are not found in nature; additional neutrons must be added to the harmonic oscillator figures (e.g., $^{40}_{40}Zr^{80}$ + the 1 g 9/2 neutron subshell = the $^{50}_{40}Zr^{90}$ 'magic' nucleus). *B* 3 depictions of one of the horizontal layers of protons (or neutrons) in the $^{40}_{40}Zr^{80}$ nucleide. Above, the principle quantum number is found to be dependent upon the radial distance from a central point. In the middle, the total angular momentum value, *j*, of a nucleon is found to be dependent upon the nucleon's radial distance from the z-axis. Below, the nucleon's magnetic moment quantum value, *m*, is found to correlate with oblique vertical planes through the lattice figures – the planes alternating between positive and negative value (darkened spheres positive, light spheres negative).

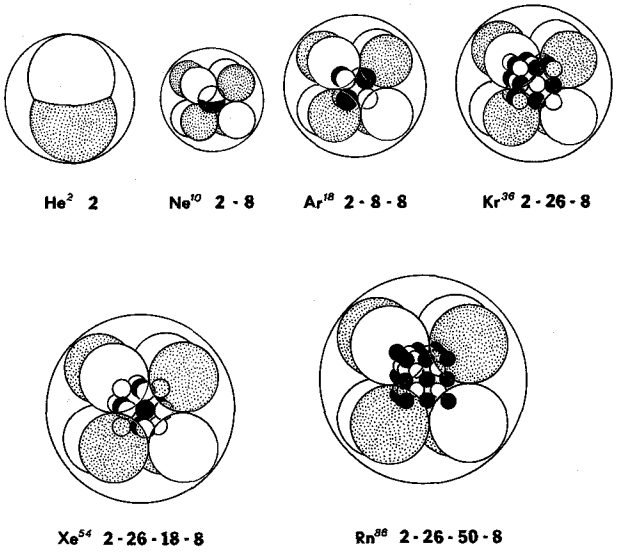

Fig. 2. The inert gas closed shells of atomic structure, drawn to approximate scale. Building from the helium shell, where the 2 electrons which straddle the nuclear charge assume roughly hemispherical volumes, cubic shell structures of 10, 18, 36, 54, and 86 electron spheres are found. The electron charge itself circulates within the electron sphere 'probability cloud' – the size of which is variable depending upon the given electron's electromagnetic environment – giving rise to a magnetic moment. Spin up electrons (magnetic north away from the nucleus) are the darkened spheres; spin down electrons are the light spheres.

and closed symmetrical ($x = y \neq z$) structures at all of the harmonic oscillator subshells. This is to say that the shell and subshell organization of the FCC lattice is identical with the harmonic oscillator shells and subshells – which are, in turn, the basis for the 'shell' or 'independent particle' theory of nuclear structure. As depicted in figure 1, the FCC build-up procedure allows for a rationalization of the basic 'liquid drop model' characteristics of nuclei (nearest neighbor nucleon interaction and the implied saturation of the nuclear force, constant nuclear density, and the dependence of nuclear radial values on the number of nucleons present) as well as rationalizing the fundamental shell-like structure of nuclei. An interesting feature of the FCC lattice is that a unique labelling system for nucleons is also implied. The principal quantum number, *n*, is found correlated with the FCC shells (figure 1, A); the angular momentum quantum number, *j*, correlates to the radial extent of the nucleon from the z-axis (in analogy with classical mechanics); and the magnetic moment quantum number, *m*, is found to relate to vertical planes through the lattice figures (figure 1, B). Spin values of the nucleons are always opposite for nearest neighbor like-fermions, implying a checkerboard pattern (figure 1, B) and alternating layers of protons and neutrons. Including the spin, isospin, angular momentum, principal, and magnetic moment quantal values, each nucleon is defined uniquely within the lattice structure[2,3]. In this model, the shells of nuclear structure are seen to be literally geometrical shells – the filling of which maximizes the 2-body nuclear bonding, thereby giving the closed shell and, to a lesser extent, closed subshell nuclei 'magic' stability.

The electron configuration, although built from the same principle of singlet pairing adjacent like-fermions, takes on a very different structure from that of the nucleus for 2 principle reasons: a) atomic structure is built of electrons with no neutral particles present, and b) rather than a homogenous nearest neighbor attraction among the particles as in the nucleus, there is a central electrostatic force which forces the electrons, despite their mutual electrostatic repulsion, into tightly packed configurations. Consequently, the adjacency of electrons is necessarily adjacency in the spherical coordinate system centered on the positive nuclear charge. Starting with 2 singlet paired electrons which, due to their electrostatic repulsion, are placed on opposite sides of the nuclear charge and building geometrical structures which conform to the principle of nearest neighbor singlet pairing, a series of closed shell symmetrical structures arise at: 2, 10, 18, 28, 36, 46, 54, 78, and 86 electrons. Of these 9 closed shell structures, 5 are found to have an external valence shell of 8 electrons, i.e., the inert noble gases; helium of course has only 2 electrons (figure 2). The remaining 3 closed shell structures which arise due to the singlet pairing of nearest neighbor electrons are found at the noble metals, Ni^{28} (shells of 2 and 26 electrons), Pd^{46} (2, 18, 26), and Pt^{78} (2, 26, 50). In other words, the principle of singlet pairing adjacent electrons produces a unique set of closed shell structures at the noble gases and noble metals. As is obvious in 3-dimensional models, all intermediate structures (e.g. octahedrons, icosahedrons, dodecahedrons, etc., all of which are non-cubic configurations) violate the principle of nearest neighbor singlet pairing.

An interesting consequence of this model building is that face centered cubic close packing of the noble gases and metals is predicted because of the cubic nature of the closed shell structures. This is in distinct contrast to quantum mechanical calculations which incorrectly predict HCP crystallization[4]. In summary, both the shell structure of the atom and the shell structure of the nucleus can be rationalized in terms of the geometrical structures which arise due to the singlet pairing of adjacent like-fermions. Previously, geometrical arguments have been used to rationalize both electron structure[5-8] and nuclear structure[9-12]. Each, however, has been a model uniquely applicable to one system or the other. On the other hand, the models for both electron and nuclear structure described above are derived from a single principle of particle interaction.

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Ceralbol, a new sesterterpenic alcohol isolated from insect wax[1]

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Summary. The isolation and structural elucidation of ceralbol (**1**), a new sesterterpene from the insect wax *Ceroplastes albolineatus* are reported.

The insect wax *Ceroplastes albolineatus* (Coccidae) was previously shown to contain a number of closely related terpenes containing 25 carbon atoms (Sesterterpenes), all of which are characterized by C_5-C_8-C_5 ring system[3-5].

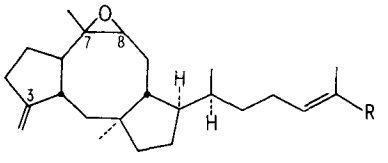
More recently the insect wax has provided 2 sesterterpenes, albocerol and albolineol, monocyclic and bicyclic respectively[6,7].

Examination of the more polar fractions of the neutral part, after saponification of this wax, has now led the isolation of a new alcohol. Here we report structural determination of this new substance, which we called ceralbol (**1**).

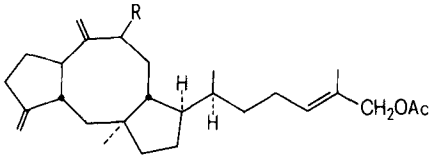
Ceralbol (**1**) is a viscous liquid, has: $[\alpha]_D + 47°$; ν_{max} 3420, 1650 and 875 cm^{-1}; λ_{max} 207 nm (ε 5800) indicating the presence of OH groups and insaturation. Its mass spectrum shows molecular ion at m/e 372 ($C_{25}H_{40}O_2$). Its NMR shows signals at δ (Me_4Si) 0.8 (3H, d, J = 6.5, sec-Me), 0.76 (3H, s, C-Me), 1.16 (3H, s, $-O-C-Me$), 1.62 (3H, s, $-C=C-Me$), 2.10 (1H, s, OH), 3.98 (2H, s, $-CH_2-OH$), 5.32 (1H, t, J = 7, $=CH-$) and 4.82 (2H, s, $=CH_2$) and its acetate (**1a**) has ν_{max} 1735 cm^{-1}, the fact that the IR spectrum of **1a** does not show OH bands suggests that the 2nd oxygen atom of ceralbol (**1**) belongs to an epoxy group. Furthermore the mass spectrum exhibits an ion at m/e 398 (M^+-16).

From its empirical formula, spectroscopic data for **1**, **1a** as well as by biogenic considerations, we decided that ceralbol must be a tricyclic compound with an epoxy group, with 2 double bonds, 1 being a terminal methylene group and the 2nd located in the side chain containing the alcohol group. We propose structure **1** from the following evidences.

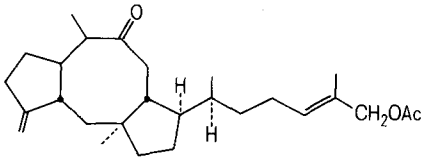
Oxidation of ceralbol (**1**) with CrO_3/piridine yielded an $\alpha\beta$ unsaturated aldehyde (**1b**) $C_{25}H_{38}O_2$ (M^+, m/e 370) ν_{max} 1680, 1630 and λ_{max} 230 nm (ε 13700) whose NMR-spectrum was almost identical to that of the parent compound apart from the signals for the proton of the aldehyde group (9.4) and the β proton on the unsaturated carbonilic system (6.37).



1- R = -CH_2OH
1a- R = -CH_2OAc
1b- R = -CH=O



2- R = -OH
2a- R = =O



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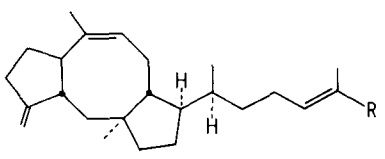

4- R = -CH_2OH
4a- R = -CH=O