functions. For the $2p^2$ configuration we need only one $\varphi_{(\alpha)}$ for the $2p$ orbital. But if the subscript p of the basis functions $\chi_{p(\alpha)}$ runs, say, from 1 to n, we are supplied with a set of orbitals $\varphi_{i(\alpha)}$ where i also runs from 1 to n and the usual procedure is that we pick up one orbital $\varphi_{i(\alpha)}$ which corresponds to the lowest "orbital energy." It is important to note that the set of orbitals $\{\varphi_{i(\alpha)}\}$ spans the same functional space as the one spanned by the original set $\{\chi_{p(\alpha)}\}$ and each member of the new set $\varphi_{i(\alpha)}$ is orthogonal to one another. Taking advantage of this property we can treat the $1s^22s^22p3p\ ^1P$ state in the following way.

(I) Apply Roothaan's SCF scheme to the $1s^22s^22p^2\ ^3P$ state. It gives a set of orthogonal functions for the p orbitals;

$$\varphi_{1(\alpha)},\ \varphi_{2(\alpha)},\ \cdots,\ \varphi_{n(\alpha)},$$

where

$$\varphi_{i(\alpha)}=\sum_{p=1}^{n}\chi_{p(\alpha)}C_{pi}.$$

Suppose that the above sequence is in the order of ascending "orbital energy." Thus $\varphi_{1(\alpha)}$ is taken for the $2p$ orbital.

(II) Now we consider the $1s^22s^22p3p\ ^1P$ state. Represent the $2p$ orbital by $\varphi_{1(\alpha)}$ and keep it fixed. Apply the SCF procedures described in the present paper to $1s^22s^23p$ by using $\varphi_{2(\alpha)}$, $\varphi_{3(\alpha)}$, $\cdots$, $\varphi_{n(\alpha)}$ as a new set of basis functions for the $3p$ orbital. Thus we get

$$\varphi_{2(\alpha)}',\ \varphi_{3(\alpha)}',\ \cdots,\ \varphi_{n(\alpha)}',$$

where

$$\varphi_{i(\alpha)}'=\sum_{p=2}^{n}\varphi_{p(\alpha)}C_{pi}'.$$

Here $\varphi_{2(\alpha)}'$ is the first approximation for the $3p$ orbital. Notice that these functions are all guaranteed to be orthogonal to the fixed $2p$ orbital $\varphi_{1(\alpha)}$.

(III) Represent the $3p$ orbital by $\varphi_{2(\alpha)}'$ and keep it fixed. Use $\varphi_{1(\alpha)}$, $\varphi_{3(\alpha)}'$, $\varphi_{4(\alpha)}'$, $\cdots$, $\varphi_{n(\alpha)}'$ as a new set of basis functions for the $2p$ orbital. Thus we get

$$\varphi_{1(\alpha)}',\ \varphi_{3(\alpha)}'',\ \varphi_{4(\alpha)}'',\ \cdots,\ \varphi_{n(\alpha)}'',$$

where $\varphi_{1(\alpha)}'$ is the second approximation for the $2p$ orbital.

(IV) Represent the $2p$ orbital by $\varphi_{1(\alpha)}'$ and keep it fixed. Use $\varphi_{2(\alpha)}'$, $\varphi_{3(\alpha)}''$, $\cdots$, $\varphi_{n(\alpha)}''$ as a new set of basis functions for the $3p$ orbital.

(V) Continue the above procedures until self-consistency is attained.

It should be admitted that the procedure described above is not at all simple and the convergence property of the whole process is not very clear mathematically. In some favorable cases, however, it could be of practical value because the number of necessary basis functions n is expected to be rather small in most cases.

V. CONCLUSION

It has been shown that with some additional elaborations Roothaan's SCF theory covers almost all the electronic configurations of atoms and molecules which are of immediate importance. It is easy to extend *formally* the SCF procedure described in the present paper in such a way that some classes of three, four or more open shells can be accommodated but it hardly seems worthwhile to make such a formal extension.

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K-Electron Capture Branch of Sr^{87m}†

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The existence of a $(0.65\pm0.25)\%$ K-electron capture branch in the decay of 2.8-hr Sr^{87m} has been established by means of an "internal source" technique. The low $\log ft=4.25$ and small energy release of 115 kev make this K branch especially interesting because it establishes Rb^{87} as a possible low-threshold detector for the inverse neutrino capture reaction, $Rb^{87}+\nu\rightarrow Sr^{87m}+e^-$, which could be identified by observing the characteristic decay of the Sr^{87m} isomer.

THE 2.8-hr Sr^{87m} isomer decays by an $M4$ transition of 388 kev to the Sr^{87} ground state. We find that it also decays by a previously undetected K-electron capture branch to Rb^{87}. From the measured ft value we can calculate the rate of the inverse reaction and thus judge the potential usefulness of Rb^{87} as a low-energy neutrino detector.

In Sr^{87m}, the 49th neutron is in a $p_{\frac{1}{2}}$ state, while in the ground state it is in a $g_{9/2}$ state. Long-lived Rb^{87} ($t_{\frac{1}{2}}\approx6\times10^{10}$ yr) decays to Sr^{87} by β^- emission, with a

† This work was performed under the auspices of the U. S. Atomic Energy Commission.

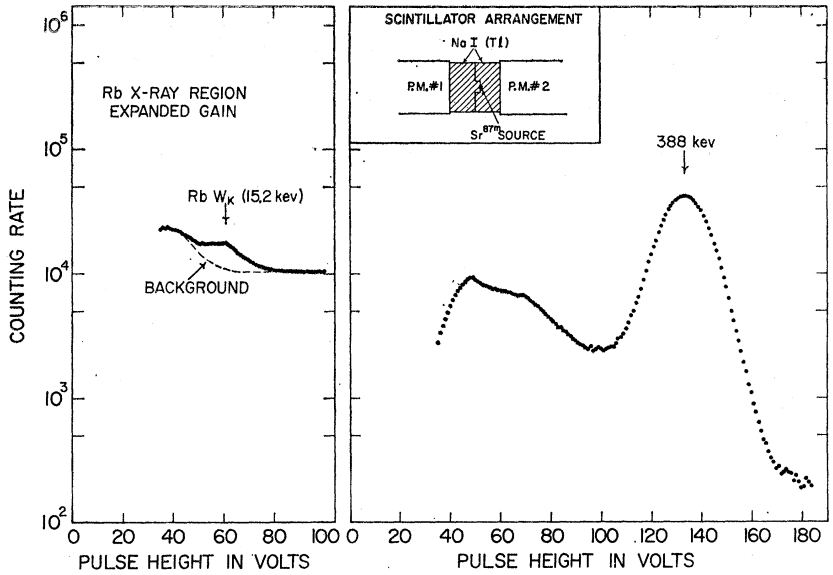

FIG. 1. Pulse-height distributions from NaI(Tl) detector in the regions of the K binding energy and the full isomeric transition energy, respectively. Insert is schematic representation of the scintillator arrangement.

maximum β-ray energy of 273 kev. Since the shell-model assignment for the 37th proton in Rb^{87} is $p_{\frac{1}{2}}$, Sr^{87m} may have an allowed K-electron capture branch to Rb^{87}, with a total energy release of 115 kev. Because of the small available energy, this branch is expected to be small and difficult to find by conventional observations. We have searched for this branch by using an "internal source" technique, in which a minute sample of Sr^{87m} was placed inside a split NaI(Tl) scintillator for 4π counting. The scintillator consisted of 2 cylindrical pieces, each $1\frac{1}{4}$ in. in diameter and $\frac{3}{4}$ in. long. The face of one piece was machined so as to have a hub $\frac{1}{2}$ in. in diameter and $\approx\frac{1}{4}$ in. in height, centered on the axis of the cylinder. This hub fits snugly into a corresponding hole in the second half of the scintillator. The source was deposited on the center of the hub. Because of optical coupling difficulties in this arrangement, two photomultipliers were used to collect the light from the composite scintillator. The photomultiplier outputs were added in a summing circuit after appropriate gain adjustments were made.

With such a source and scintillator arrangement, no K x rays arising from conversion of the isomeric transition can be detected as an isolated peak, since the accompanying conversion electron is simultaneously detected with unit efficiency. The signal from the scintillator always corresponds to the full isomeric transition energy. The isomeric transitions which take place by γ emission are detected by the counter in the usual way. One observes a Compton distribution, and a photopeak coinciding with the full energy peak in the conversion electron case. However, when a K-shell vacancy is created by a competing K-electron capture process, the signal from the detector now corresponds to detection of an energy equal to the K-shell binding energy in the daughter atom, and one observes a photopeak at this energy. The magnitude of the K-electron capture branch is determined by the ratio of events in the "K" photopeak to events arising from the isomeric transition, when the appropriate correction for γ-ray detection efficiency is made.

Figure 1 shows the observed pulse-height distribution of signals from the detector, as recorded by a multichannel analyzer. The K binding energy region and the full isomeric transition energy region were run at different amplifier gains, and for different counting times.

In computing the magnitude of the K-electron capture branch, it was necessary to estimate the efficiency for detecting the isomeric transition for our particular arrangement of source and scintillation counter. For this purpose we take the total conversion coefficient for the isomeric transition as 0.28.[1] The conversion electrons are detected with unit efficiency. The remaining 78% of the isomeric transitions take place by γ emission. We estimate that 34% of these γ transitions are detected in the full-energy peak. Thus,

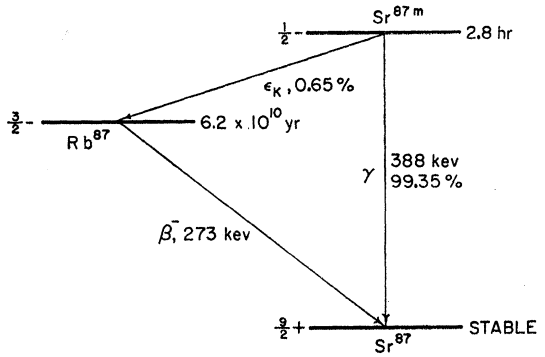

FIG. 2. Sr^{87m} decay scheme.

[1] L. G. Mann and P. Axel, Phys. Rev. 84, 221 (1951).

our over-all efficiency for detecting the isomeric transitions in the full-energy peak is $\epsilon_{I.T.}=0.22\times1+0.78\times0.34=0.485$. After making the appropriate corrections for decay between the two runs, and for counting time and efficiency, we find the ratio

$$(K \text{ capture})/(\text{isomeric transitions})=(6.5\pm2.5)\times10^{-3}.$$

The resulting decay scheme is shown in Fig. 2. If we take the energy available in K capture as 115 kev, we find $\log ft\cong4.25$ for the K-electron capture branch. This small ft value is consistent with ft values for other allowed K capture and β-decay ft values for nuclei at closed shells, where a nucleus with a single "hole" makes a transition to a nucleus with a closed shell.[2]

The presence of the allowed K-electron capture branch with a small ft value in the Sr^{87m} decay, together with the small (115 kev) energy release in the K-capture process, makes it interesting to speculate about the possibility of observing the inverse neutrino capture reaction, $Rb^{87}+\nu\rightarrow Sr^{87m}+e^-$. This reaction could in principle be identified by observing the characteristic isomeric transitions of Sr^{87m} chemically extracted from a Rb sample exposed to a neutrino flux, e.g., from the sun. In order to estimate the yield from this reaction, it is necessary to average the neutrino capture cross section over the incoming neutrino energy distribution. According to current ideas[3] about energy production in the sun, about $\frac{2}{3}$ of the neutrinos from the sun have their origin in the reaction

$$p+p\rightarrow d+\nu+e^+,$$

while the remaining $\frac{1}{3}$ arise from electron capture in Be^7. Of this latter group, 88% originate from the transition to the ground state of Li^7 while 12% come from electron capture to the 477-kev excited state of Li^7. Thus, the major portion of the neutrino flux from the sun consists of the continuous energy distribution from the $p+p$ capture reaction ($E_{max}=421$ kev), and two essentially monoenergetic neutrino groups at 386 kev and 863 kev. The intensities are in the ratio 100:6:44, respectively.

The neutrino capture cross section as a function of incoming neutrino energy is given by

$$\sigma=4\pi\lambda_K\frac{E_e^2}{E_\nu^2}\frac{(P_e/E_e)F(Z,E_e)}{g_K^2(R)}\frac{(\hbar/mc)^2}{(mc^2/\hbar)}S.$$

Here λ_K is the decay constant for the K capture process in sec^{-1}, E_ν is the energy (in units of mc^2) of the neutrino emitted in the K capture process, E_e is the energy (in units of mc^2) of the outgoing electron, p_e is the electron momentum (in units of mc), g_K is the radial wave function for the K electron, $F(Z,E_e)$ is the Fermi function, and S is the statistical weight factor in the neutrino capture reaction.

When this cross section is averaged over the incoming neutrino energy distribution, we find $\bar{\sigma}=1.2\times10^{-45}$ cm^2. If we assume an integrated neutrino flux from the sun equal to $\sim10^{11}/\text{cm}^2$ sec, this cross section implies a rate of production of Sr^{87m} equal to ~1 per min in 10^5 tons of normal rubidium.

One may alternatively adopt the attitude that the neutrino flux in our environment is unknown, and that it is worthwhile to set an upper limit on its value by attempting to observe this reaction on a small scale. We have performed this simple experiment by counting on a well-shielded 3-in. $\times$3-in. NaI(Tl) scintillation counter the Sr fraction chemically separated from 30 grams of rubidium fluoride, searching for the 388-kev γ ray in the Sr^{87m} decay. Our experimental upper limit on the number of 388-kev photons emerging from the Sr fraction leads us, again assuming an average cross section $\bar{\sigma}=1.2\times10^{-45}$ cm^2, to an upper limit for the number of neutrinos with energies appreciably above the threshold for the Rb^{87} reaction, which is $\lesssim2.2\times10^{21}/\text{cm}^2$ sec.

Recently possible experiments on the limits of breakdown of electric charge conservation were discussed.[4] It may be worth noting that the experiment described here also sets a lower limit on the lifetime for possible nonconservation of electric charge of nucleons.[5]

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[2] A. de-Shalit and M. Goldhaber, Phys. Rev. **92**, 1211 (1953).

[3] E. Burbidge, G. R. Burbidge, W. A. Fowler, and F. Hoyle, Revs. Modern Phys. **29**, 547 (1957).

[4] G. Feinberg and M. Goldhaber, Proc. Natl. Acad. Sci. U. S. **45**, 1301 (1959).

[5] Suppose that a neutron in Rb^{87} changes spontaneously into a proton by emitting, for example, a neutrino pair. Since, unlike in ordinary β decay, no electron mass is involved, this process can lead to Sr^{87m} with an energy release of 396 kev, which is shared between the neutrinos. Our failure to observe the Sr^{87m} isomeric transition in the sample separated from RbF sets a lower limit on the mean life for this process at $\tau\gtrsim1.8\times10^{16}$ yr, if we assume that only a single neutron in Rb^{87} can contribute to this process.