ditional form for a configuration in which all singly occupied orbitals have parallel spin. This of course would require iterated energy band calculations, with inclusion of exchange, by the self-consistent field method, but it is probably not unreasonable to hope for such results in the foreseeable future. Then the occupied orbitals (calculated as Bloch waves) should be transformed to the equivalent set of Wannier functions,[19] localized as much as possible on single atoms in the crystal. The singly occupied Wannier functions on each atom should be occupied with parallel spin. The various contributions to the Heisenberg exchange integral can then be evaluated by the formulas given in the present paper. These formulas depend for their validity only on the orthogonality of the spatial orbitals, which is maintained by the unitary transformation from Bloch waves to Wannier functions. For metals this procedure would in some cases have to be modified to account for partially filled bands by introducing an appropriate sublattice structure, as described in an earlier paper.[4]

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The calculations reported in this paper were carried out on the IBM 704 computer, using a package of computer programs for molecular calculations programmed by the author. The program for matrix self-consistent field calculations by the method of Roothaan [C. C. J. Roothaan, Revs. Modern Phys. **23**, 69 (1951)] as modified by the author [R. K. Nesbet, Mass. Inst. Technol. Quart. Prog. Rept., Solid State and Molecular Theory Group, October 15, 1955, pp.4–8 (unpublished)] and the program for data retrieval were coded at the National Bureau of Standards by A. Beam, P. Walsh, and J. D. Waggoner, under the supervision of Dr. E. Haynesworth. The programs for evaluation of two-center integrals were coded by the author [R. K. Nesbet, Revs. Modern Phys. **32**, 272 (1960)] using methods developed by P. Merryman. This work was supported by RIAS.

The programs used were tested by the usual internal checks, and also in detail against the earlier calculations on N_2 by Scherr (reference 8). Errors of a numerical nature are expected to affect the results quoted here at most in the fourth figure after the decimal point.

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Nonexistence of a 9.0-Mev Level in C^{12}†

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An energy level in C^{12} at 9.0 Mev has been reported as a result of (p,γ,γ) triple coincidence measurements on the $B^{10}(He^3,p)C^{12}$ reaction at $E_{He^3}=2.2$ Mev. This reaction has been reinvestigated in a similar experimental arrangement by using alternately Pilot-*B*, CsI and NaI scintillators for detection of the protons. Only the Pilot-*B*, which had been used in the previous work, exhibits the proton group corresponding to a "9.0-Mev level" in C^{12}. The triple coincidence effect in this case is actually due to the intense ~17-Mev protons in the $B^{10}(He^3,p)C^{12}$ reaction leading to the 4.43-Mev first excited state of C^{12} which upon entering the scintillator can inelastically scatter from carbon and produce secondary gamma radiation of 4.43 Mev. The net energy deposited in the scintillator has the appearance of a proton group to a 9.0-Mev level in C^{12} in triple coincidence with two 4.43-Mev gamma rays. The magnitude of the effect is calculated from published cross sections for inelastic scattering and it agrees with the apparent population intensity of the nonexistent "9.0-Mev level."

A CONSIDERATION of possible gamma-ray background effects when using plastic scintillators for the detection of energetic protons has led us to a reinvestigation of the $B^{10}(He^3,p)C^{12}$ reaction. (p,γ,γ) triple coicidence measurements[1] had suggested the existence of a weakly populated energy level in C^{12} at 9.0 Mev. In these experiments the protons were detected in a Pilot-*B* scintillator close to the target which accepted protons emitted in the angular range 0°–60° and the gamma rays were detected in two large NaI

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detectors placed closely on either side of the target. When both NaI detectors were channeled on gamma rays between 2.5 and 5 Mev, a proton "group" was observed in triple coincidence having an energy corresponding to a level in C^{12} at 9.0 ± 0.1 Mev.

Since the Q value of the $B^{10}(He^3,p)C^{12}$ reaction is high (19.70 Mev to the ground state), inelastic scattering of the protons from nuclei in the scintillation detector might be an observable effect. In particular the protons leading to the 4.43-Mev first excited state of C^{12} have an energy of 17.3 Mev at 0° and 16.4 Mev at 60° when $E_{He^3}=2.2$ Mev. If these protons inelastically scatter in a scintillator containing carbon, secondary gamma rays of 4.43 Mev are produced when the scattering takes place to the first excited state of C^{12}. This results in real triple coincidence events in which the net energy deposited by the proton is approximately 4.4 Mev less than the energy of the proton group to the 4.43-Mev state in the initial reaction. The recoil effect of the inelastic scattering tends to lower the pulse height somewhat if the scintillator is less efficient in responding to the C^{12} recoil nucleus.

In Fig. 1 the probability of producing a 4.43-Mev gamma ray by inelastic scattering in a plastic detector is plotted versus incident proton energy. It is assumed that the detector has an atomic ratio $C/H=0.89$ and is thick enough to absorb the protons. The curve is calculated from experimentally determined cross sections[2–7] for the reaction $C^{12}(p,p')C^{12}{}_{4.43}$. The relative accuracy in the probability is low at low proton energies and is roughly constant at about $\pm0.2\times10^{-3}$ above a proton energy of 10 Mev. At a proton energy of 16.9 Mev, which is the average energy for emission between 0° and 60° of protons leading to the 4.43-Mev state in the $B^{10}(He^3,p)C^{12}$ reaction at $E_{He^3}=2.2$ Mev, the probability is 2.1×10^{-3} per proton. This value is in agreement with the apparent branching ratio[1] of $(2.1\pm0.7)\times10^{-3}$ for protons leading to a "9.0-Mev level" relative to those leading to the 4.43-Mev level.

Our present experimental arrangement was essentially the same as that used earlier.[1] When Pilot-B is employed as the proton detector the proton line to the "9.0-Mev level" is observed in triple coincidence with the two gamma-ray detectors, but when either CsI or NaI are used for proton detection the corresponding region of the pulse-height curve is flat and is smaller by at least a factor of 10 as compared with the peak observed in the Pilot-B runs.

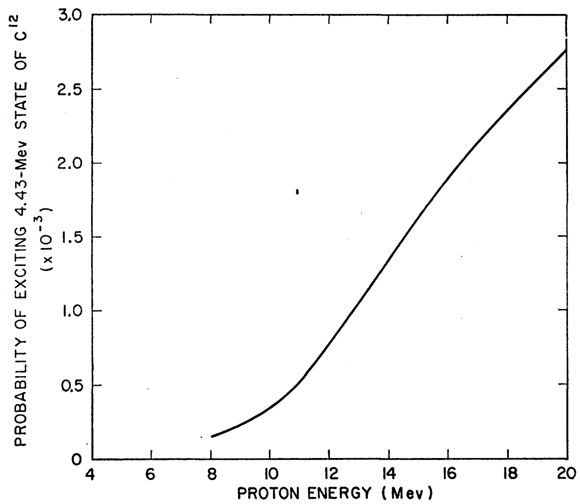

FIG. 1. The probability of exciting the 4.43-Mev first excited state of C^{12} by the reaction $C^{12}(p,p')C^{12}{}_{4.43}$ for protons completely absorbed in a plastic scintillator of composition $C/H=0.89$.

We conclude that the apparent 9.0-Mev level is a result of the instrumental effect described above and that no such energy level exists in C^{12}.

The $B^{10}(He^3,p)C^{12}$ reaction was investigated[1] originally in an attempt to detect the emission of 3.2-Mev gamma radiation from the 7.66-Mev second excited state of C^{12}. Proton inelastic scattering effects of the type discussed above may preclude the use of this reaction in such a (p,γ,γ) coincidence experiment. From the ratio of 4×10^{-2} for the branching intensity of protons to the 7.66-Mev state relative to the protons to the 4.43-Mev state at $E_{He^3}\sim2$ Mev and from the estimate[8,9] of $\sim2\times10^{-4}$ for the 3.2-Mev gamma-ray decay per 7.66-Mev level formed, the (p,γ,γ) triple cascade rate associated with the 7.66-Mev state is estimated to be $\sim8\times10^{-6}$ with respect to the protons to the 4.43-Mev state. This number is 250 times smaller than the triple coincidence yield of 2×10^{-3} observed with the Pilot-B detector and thus a reduction of the inelastic scattering effect by at least two orders of magnitude would have to be achieved in order for the gamma-ray decay of the 7.66-Mev level to be observed. Such a reduction might be brought about by degrading the proton energies and by using a suitable scintillation material, although the background effects from the proton absorber or target backing may be limitations to this scheme.

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