Evidence for Triangular D'_{3h} Symmetry in ^{13}C

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We derive the rotation-vibration spectrum of a $3\alpha + 1$ neutron(proton) configuration with triangular D_{3h} symmetry by exploiting the properties of the double group D'_{3h} and show evidence for this symmetry to occur in the rotation-vibration spectra of ^{13}C. Our results, based on purely symmetry considerations, provide benchmarks for microscopic calculations of the cluster structure of light nuclei.

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The cluster structure of light nuclei is a long-standing problem that goes back to the early times of nuclear physics [1]. Recently, there has been renewed interest in this problem due to new measurements in ^{12}C [2–5], showing evidence for the occurrence of D_{3h} triangular symmetry in this nucleus. Most applications of cluster models has been so far limited to $k\alpha$ nuclei, that is nuclei composed of k α particles, with $k = 2, 3, 4$, which display Z_2 (^{8}Be), D_{3h} (^{12}C), and T_d (^{16}O) symmetry [6,7]. Study of structures composed of k α particles plus x additional nucleons, simply denoted here by $k\alpha + x$ nuclei, has been hindered by the lack of understanding of the single-particle motion in an external field with arbitrary discrete symmetry, G, and, especially, by the lack of explicit construction of representations of the double group, G', which allows the enlargement of tensor (bosonic) representations of the group G to cases in which there is one fermion, the so-called spinor (fermionic) representations. Recently, we have started a systematic investigation of both problems. The study of the splitting of single-particle levels in an external field with Z_2, D_{3h}, and T_d symmetry was carried out in Ref. [8]. The construction of representations of the double group Z'_2 is trivial because the 2α structure possessing this symmetry is a dumbbell configuration with axial symmetry [9]. The construction of representations of the double groups D'_{3h} and T'_d is more complicated. Although done for applications to crystal physics by Koster *et al.* [10] and molecular physics by Herzberg [11], to the best of our knowledge, it has never been done for applications to nuclear physics. In this Letter, we report the results of our investigation of the double group D'_{3h} and, in an application to the nucleus ^{13}C, we present evidence for the occurrence of D'_{3h} symmetry in nuclear physics.

The double group D'_{3h} has three spinor representations, denoted by Koster as Γ_7, Γ_8, Γ_9 [10] and by Herzberg as $E_{1/2}$, $E_{5/2}$, $E_{3/2}$ [11]. We prefer, for applications to nuclear physics, to denote the three representations by $E^{(+)}_{1/2} \equiv \Gamma_7 \equiv E_{1/2}$, $E^{(-)}_{1/2} \equiv \Gamma_8 \equiv E_{5/2}$, $E_{3/2} \equiv \Gamma_9 \equiv E_{3/2}$, and label the states by $|\Omega, K, J\rangle$, where Ω labels the representations of D'_{3h}, and K and J are half integers representing the projection K of the total angular momentum J on a body-fixed axis. The allowed values of K^P for each one of the spinor representations are given by

$$\begin{array}{llll}
\Omega = E^{(+)}_{1/2}: & K^P = 1/2^+ \quad \text{and} & & \\
& K = 3n \pm \frac{1}{2} & P = (-)^n & \\
\Omega = E^{(-)}_{1/2}: & K^P = 1/2^- \quad \text{and} & & \\
& K = 3n \pm \frac{1}{2} & P = (-)^{n+1} & \\
\Omega = E_{3/2}: & K^P = (3n - \frac{3}{2})^\pm & , &
\end{array} \tag{1}$$

with $n = 1, 2, 3, \ldots$, and $K > 0$. The angular momenta of each K band are given by $J = K, K + 1, K + 2, \ldots$. Note the double degeneracy $K^P = K^\pm$ for the representation $E_{3/2}$ (parity doubling).

This classification allows one to construct the rotational spectrum of a triangular configuration of three α particles dragging along an additional proton or neutron. The rotational formula is

$$E_{\rm rot}(\Omega, K, J) = \varepsilon_\Omega + A_\Omega[J(J+1) + b_\Omega K^2 + a_\Omega g_\Omega(J)], \tag{2}$$

where ε_Ω is the intrinsic energy [8], $A_\Omega = \hbar^2/2\Im$ is the inertial parameter, b_Ω is a Coriolis term, and a_Ω is the so-called decoupling parameter with $g_\Omega(J) = \delta_{K,1/2}(-1)^{J+1/2}(J + 1/2)$. The latter term applies only to representations $\Omega \equiv E^{(\pm)}_{1/2}$ and $K^P = 1/2^\pm$.

The rotational spectra of ^{13}C are shown in Fig. 1 where the experimental levels are plotted as a function of $J(J+1)$. The ground state band has $K^P = 1/2^-$ and it

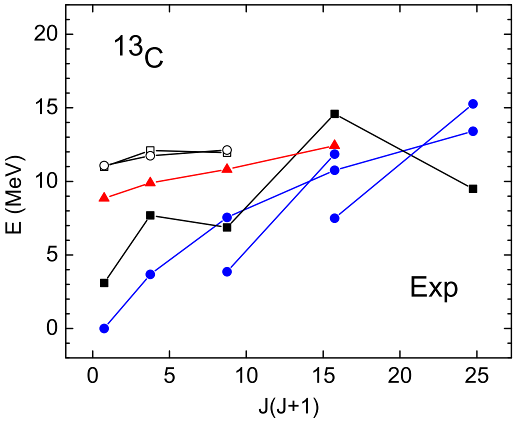

FIG. 1. The rotational spectra of ^{13}C. Energy levels [15] are plotted as a function of $J(J+1)$. For states below 10 MeV, our assignment of rotational bands is unambiguous. For states above 10 MeV, our assignment is tentative.

can be assigned to the representation $\Omega = E^{(-)}_{1/2}$ of D'_{3h} (blue lines and filled circles). As seen from Eq. (1), this representation contains also $K^P = 5/2^+$ and $7/2^+$ bands. Both of them appear to be observed as shown in Fig. 2. The observation of low-lying positive parity states with $K^P = 5/2^+$ and $7/2^+$ is crucial evidence for the occurrence of D'_{3h} symmetry. In the shell model, positive parity states are expected to occur at much higher energies because they come from the $s-d$ shell. They were not considered in the original calculation of Cohen and Kurath [12]. In more recent calculations which include $(0s)^3(1p)^{10}$ plus $(0s)^4(1p)^8(2sd)^1$ configurations, they are brought down by lowering the energy of the $2s_{1/2}$ level from 11 to 5.43 MeV [13] or 5.52 MeV [14], and by adjusting the p-h interaction [13].

The first excited rotational band has $K^P = 1/2^+$. It can be assigned to the representation $\Omega = E^{(+)}_{1/2}$ of D'_{3h} (black line and filled squares). This band has a large decoupling parameter, $a_\Omega = 1.24$. According to Eq. (1), this representation contains also $K^P = 5/2^-$ and $K^P = 7/2^-$ bands. The evidence for these bands is meager, because they are expected to lie at high energy. There is some tentative evidence for the $K^P = 5/2^-$ band at energies > 15 MeV, but no evidence for the $K^P = 7/2^-$. This appears to indicate that the Coriolis coefficient b_Ω is less negative than that of the $E^{(-)}_{1/2}$ band (or even positive). Assuming a value of $b_{1/2^+} = 0.80$, we calculate the $K^P = 5/2^-$ bandhead at ∼13 MeV and the $K^P = 7/2^-$ bandhead at ∼20 MeV. This situation is shown in Fig. 3.

The experimental value of the energy difference $E(1/2^+_1) - E(1/2^-_1) = 3.089$ MeV is further evidence of D'_{3h} symmetry in ^{13}C. From Fig. 11 of Ref. [8], we can estimate this value to be ∼2.0 MeV. Again, in the shell model the $1/2^+$ state comes from the s-d shell and is brought down by the lowering of the $2s_{1/2}$ level as mentioned in the paragraph above.

The expected vibrational spectra can be obtained by coupling the representations of the fundamental vibrations of the triangular configuration with symmetry A'_1 and E' [16,17] to the intrinsic states with $E^{(-)}_{1/2}$ and $E^{(+)}_{1/2}$ symmetry. From the multiplication table of D'_{3h}, one obtains [10,11]

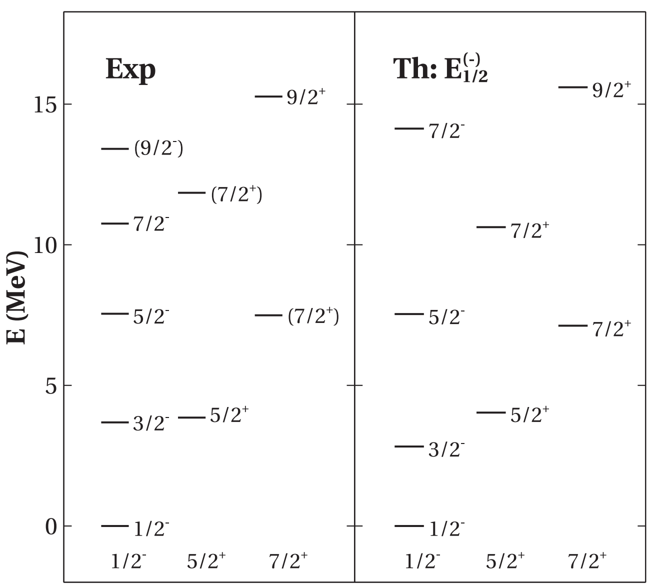

FIG. 2. Comparison between experimental and theoretical energies for the ground state band assigned to the representation $\Omega = E^{(-)}_{1/2}$ of D'_{3h}. The values of K^P are given at the bottom of the figure. The energies are calculated using Eq. (2) with $A_\Omega = 0.942$ MeV, $b_\Omega = -0.62$, and $a_\Omega = 0$.

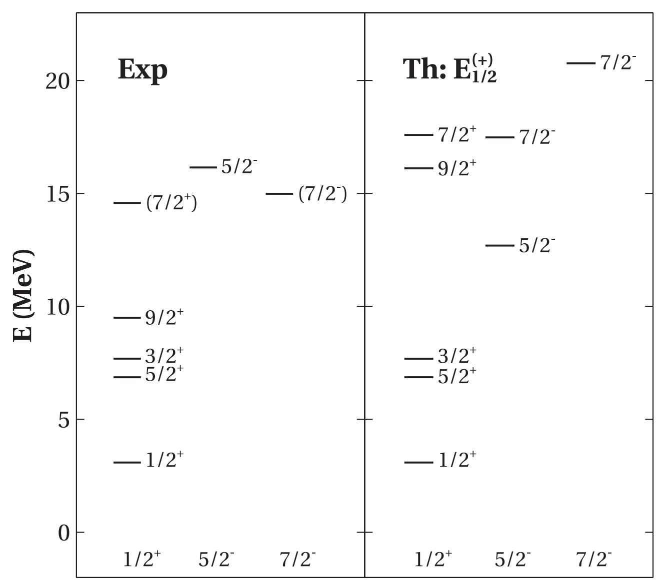

FIG. 3. As Fig. 2, but for the first excited band assigned to the representation $\Omega = E^{(+)}_{1/2}$ of D'_{3h}. The energies are calculated using Eq. (2) with $A_\Omega = 0.684$ MeV, $b_\Omega = 0.80$, $a_\Omega = 1.24$, and $\varepsilon = 3.848$ MeV.

$$A'_1 \otimes E^{(\pm)}_{1/2} = E^{(\pm)}_{1/2},$$
$$E' \otimes E^{(\pm)}_{1/2} = E_{3/2} \oplus E^{(\mp)}_{1/2}. \quad (3)$$

For each intrinsic state, one expects three states, $\Omega = E^{(-)}_{1/2}$, $E_{3/2}$, $E^{(+)}_{1/2}$ for the intrinsic state with $E^{(-)}_{1/2}$ symmetry, and $\Omega = E^{(+)}_{1/2}$, $E_{3/2}$, $E^{(-)}_{1/2}$ for $E^{(+)}_{1/2}$. We denote the corresponding vibrational quantum numbers by $v_{1\Omega}$, $v_{2\Omega}$, $v_{3\Omega}$, respectively, where, for simplicity of notation, we have omitted the label of the vibronic angular momentum l. In the analysis of the vibrational states, it is convenient to remove the zero-point energy. The vibrational formula, to lowest order in the vibrational quantum numbers (harmonic limit), is

$$E_{vib}(\Omega; v_{1\Omega}, v_{2\Omega}, v_{3\Omega}) = \omega_{1\Omega} v_{1\Omega} + \omega_{2\Omega} v_{2\Omega} + \omega_{3\Omega} v_{3\Omega}. \quad (4)$$

The vibration A'_1 in ^{12}C plays an important role in nuclear astrophysics because it is associated with the so-called Hoyle state. According to Eq. (3), we expect Hoyle states also in ^{13}C. Indeed, the Hoyle band built on top of the ground state $E^{(-)}_{1/2}$ representation appears to have been observed in ^{13}C starting at an energy of 8.860 MeV (red line and filled triangles in Fig. 1), which is slightly higher than that of the Hoyle state in ^{12}C (7.654 MeV). The moment of inertia of this band is similar to that of the Hoyle band in ^{12}C, which is further evidence for the occurrence of D'_{3h} symmetry in ^{13}C. In Fig. 1, one can also observe two additional bands with $K^P = 1/2^+$ and $K^P = 1/2^-$ starting at 10.996 MeV and 11.080 MeV. Because many states with these values of K^P are expected in this region, no firm assignments can be made, but it is very likely that these bands are the vibrations $E^{(+)}_{1/2}$ and $E^{(-)}_{1/2}$ of Eq. (3).

In the region $E \sim 10$ MeV, one expects additional rotational bands. Evidence for two rotational bands with $K^P = 3/2^\pm$ has been reported [18], starting at 9.90 MeV ($3/2^-$) and 11.08 MeV ($3/2^+$), respectively. These bands can be assigned to the representation $\Omega = E_{3/2}$ of D'_{3h} [see Eq. (1)] and split into its two components by Coriolis and other interactions. These bands were suggested to arise from ^{9}Be + α configurations [19]. A discussion of these bands will be presented in a longer publication.

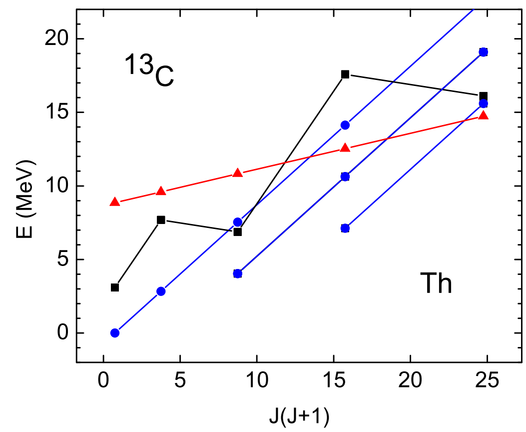

FIG. 4. Rotational spectra in ^{13}C expected on the basis of D'_{3h} symmetry.

The situation for rotational and vibrational bands in ^{13}C is summarized in Fig. 4. A comparison with the experimental spectrum in Fig. 1 shows evidence for D'_{3h} symmetry in ^{13}C.

Further evidence for the occurrence of D'_{3h} symmetry in ^{13}C is provided by electromagnetic transition rates and form factors in electron scattering. A complete analysis of electromagnetic transition rates and electromagnetic form factors in electron scattering requires an elaborate calculation similar to that done for ^{9}Be and ^{9}B in Ref. [9]. Here we limit ourselves to the most important points.

$B(E\lambda)$ values in $k\alpha + x$ nuclei can be calculated using Eq. (25) of [9] as

$$B(E\lambda; \Omega', J', K' \to \Omega, J, K) = |\langle J', K', \lambda, K - K' | J, K\rangle [\delta_{v,v'} G_\lambda(\Omega, \Omega') + \delta_{\Omega,\Omega'} G_{\lambda,c}] + (-)^{J+K} \langle J', K', \lambda, -K - K' | J, -K\rangle [\delta_{v,v'} \tilde{G}_\lambda(\Omega, -\Omega') + \delta_{\Omega,-\Omega'} G_{\lambda,c}]|^2. \quad (5)$$

Here $G_\lambda(\Omega, \Omega')$ represents the contribution of the single particle and $G_{\lambda,c}$ the contribution of the cluster. In ^{13}C, the single particle is a neutron and thus it does not contribute to electric transitions, except for $E1$ transitions affected by the center-of-mass correction as discussed in Eq. (32) of [9]. The cluster contribution is given by the D_{3h} symmetry as [17]

$$G_{\lambda,c} = Z\beta^\lambda \sqrt{\frac{2\lambda + 1}{4\pi}} c_\lambda, \quad (6)$$

where the coefficients c_λ are given by $c_0 = 1$, $c_2 = 1/2$, $c_3 = \sqrt{5/8}$, and $c_4 = 3/8$. The value of β extracted from the minimum in the elastic form factor of ^{12}C is $\beta = 1.74$ fm. With this value we calculate the $B(E\lambda)$ values given in Table I, where they are compared with experiment. Both experimental and theoretical values in ^{12}C show that both states, 2^+_1 and 3^-_1 belong to the same rotational band of the triangle [17], representation A'_1 of D_{3h}. Note in particular the large $B(E3)$ value that cannot be obtained in shell-model calculations without the introduction of large effective charges. Similarly, the values in ^{13}C show that the states $3/2^-_1$, $5/2^-_1$, and $5/2^+_1$ belong to the same rotational band with $\Omega = E^{(-)}_{1/2}$. Note also here the large $B(E3; 5/2^+_1 \to 1/2^-_1)$

TABLE I. $B(\mathrm{EL})$ values in ^{12}C and ^{13}C in W.U. [15].

	$B(\mathrm{EL})$	Exp	Th
^{12}C	$B(E2;2_1^+ \to 0_1^+)$	4.65 ± 0.26	4.8
	$B(E3;3_1^- \to 0_1^+)$	12 ± 2	7.6
^{13}C	$B(E2;3/2_1^- \to 1/2_1^-)$	3.5 ± 0.8	4.8
	$B(E2;5/2_1^- \to 1/2_1^-)$	3.1 ± 0.2	3.2
	$B(E3;5/2_1^+ \to 1/2_1^-)$	10 ± 4	4.3

value. This value is obtained in the cluster calculation without the use of effective charges.

In the same way, form factors in electron scattering can be split into a single-particle and collective cluster contribution, $F(q) = F^{s.p.}(q) + F^{c}(q)$, as discussed in Sec. 3.6 of Ref. [9]. For odd-neutron nuclei, the single particle does not contribute appreciably, except for multipolarity $E1$. The cluster contribution to the longitudinal electric form factors can be written as in Eq. (46) of Ref. [9]

$$F_\lambda^c(q;J,K \to J',K') = \delta_{K,K'} Z \sqrt{\frac{2\lambda+1}{4\pi}} c_\lambda \langle J,K,\lambda,0|J',K'\rangle j_\lambda(q\beta) e^{-q^2/4\alpha}, \quad (7)$$

where $\alpha = 0.56\ \mathrm{fm}^{-2}$ is obtained from electron scattering in ^{4}He and $\beta = 1.74$ fm from electron scattering in ^{12}C. Using Eq. (7), one can calculate all longitudinal form factors in a parameter independent way. The longitudinal form factors of the states $5/2_1^-$ and $3/2_1^-$ of the ground-state rotational bands are shown in Fig. 5 where they are compared with experimental data [20]. An important consequence of the cluster model is that the two form factors $1/2_1^- \to 3/2_1^-$ and $1/2_1^- \to 5/2_1^-$ have identical shapes and identical $B(E2;\uparrow)$ values: 9.6 W.U. This is to a very good approximation seen in Fig. 5.

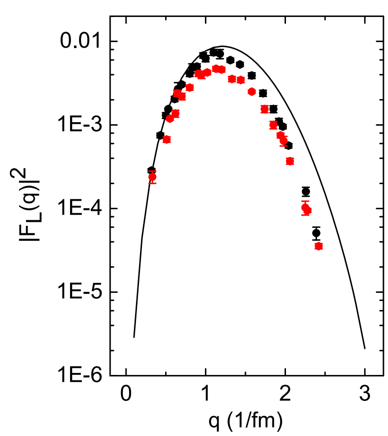

FIG. 5. Comparison between calculated and experimental [20] longitudinal $E2$ form factors for the ground-state band of ^{13}C, $1/2_1^- \to 5/2_1^-$ (black) and $1/2_1^- \to 3/2_1^-$ (red).

The discrepancy at large momentum transfer is due to the fact that the value of β appropriate to ^{12}C has been used to make the calculation parameter free. A small renormalization of this value to $\beta = 1.82$ fm reproduces the data perfectly.

In conclusion, both the rotation-vibration spectra and the electromagnetic transition rates in ^{13}C show strong evidence for the occurrence of D'_{3h} symmetry. The final picture that emerges from our analysis is that the nucleus ^{13}C can be considered as a system of three α particles in a triangular configuration plus an additional neutron moving in the deformed field generated by the cluster, as schematically shown in Fig. 6.

Details of our study of D'_{3h} as well as results for T'_d will be reported in future publications.

Finally, an important question is the extent to which the cluster structure of ^{13}C emerges from microscopic calculations. This nucleus has been extensively investigated in the shell model [13,14,20] where, however, the cluster features are obtained by adjusting the single-particle energies, the p-h interactions, and the effective charges. In recent years, fermion molecular dynamics [21–24] and antisymmetric molecular dynamics [25,26] have provided very detailed and accurate descriptions of light nuclei which confirm the cluster structure of ^{12}C and ^{13}C obtained from D_{3h} and D'_{3h} symmetry (see, for example, Fig. 10 of Ref. [24]). Very detailed calculations have also been done within the framework of the full four-body $3\alpha + n$ model [27] (this reference includes a complete list of microscopic calculations of ^{13}C). It would be of great interest to understand whether the cluster structure of ^{12}C and ^{13}C emerges from *ab initio* calculations, such as the no-core shell-model methods [28–30] for which calculations are planned. The results presented here, based on purely symmetry concepts, provide benchmarks for microscopic studies of cluster structure of light nuclei.

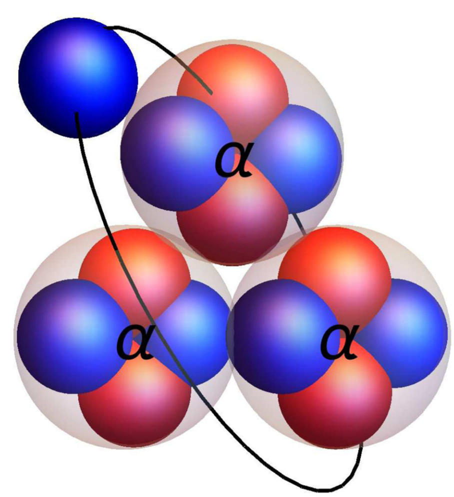

FIG. 6. Molecularlike picture of ^{13}C.

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