Evidence for Tetrahedral Symmetry in ^{16}O

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We derive the rotation-vibration spectrum of a 4α configuration with tetrahedral symmetry $\mathcal{T}_d$ and show evidence for the occurrence of this symmetry in the low-lying spectrum of ^{16}O. All vibrational states with A, E, and F symmetry appear to have been observed as well as the rotational bands with $L^P = 0^+$, 3^-, 4^+, 6^+ on the A states and part of the rotational bands built on the E, F states. We derive analytic expressions for the form factors and $B(EL)$ values of the ground-state rotational band and show that the measured values support the tetrahedral symmetry of this band.

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The cluster structure of light nuclei is a long-standing problem that goes back to the early days of nuclear physics [1]. Recent experimental developments have shown that the low-lying states of ^{12}C can be described as the rotation-vibration of a 3α cluster with $\mathcal{D}_{3h}$ symmetry (equilateral triangle) [2–5]. Departures from a rigid cluster structure appear to be moderate in size and can be accounted for by perturbation theory. In this Letter, we show that the low-lying states of ^{16}O can be described as the rotation-vibration of a 4α cluster with $\mathcal{T}_d$ symmetry (tetrahedral). The suggestion that ^{16}O has a tetrahedral 4α structure goes back many years [6–10]. However, clear signatures could not be identified. We take advantage of the algebraic cluster model (ACM) [11,12] to produce the rotation-vibration spectrum of an object with $\mathcal{T}_d$ symmetry and compare it with the observed spectrum. We also derive an analytic expression for the $B(EL)$ values along the ground-state rotational band. A comparison with the experimental values of the energy spectrum and electromagnetic transitions provides strong evidence for tetrahedral symmetry in ^{16}O.

The algebraic cluster model is a description of cluster states as representations of a $U(\nu+1)$ group where ν is the number of space degrees of freedom [11,12]. In Refs. [11,12], we described three-body clusters, where the number of degrees of freedom (after removal of the center of mass) is $\nu = 3n-3 = 6$, in terms of the algebra of $U(7)$. The space degrees of freedom there are the Jacobi coordinates $\vec{\rho} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2}$ and $\vec{\lambda} = (\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)/\sqrt{6}$, where $\vec{r}_i$ are the coordinates of the three α particles ($i = 1, 2, 3$). We describe four-body clusters with $\nu = 3n-3 = 9$ in terms of the algebra of $U(10)$. The space degrees of freedom here are three Jacobi vectors, $\vec{\rho} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2}$, $\vec{\lambda} = (\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)/\sqrt{6}$, and $\vec{\eta} = (\vec{r}_1 + \vec{r}_2 + \vec{r}_3 - 3\vec{r}_4)/\sqrt{12}$, where $\vec{r}_i$ are the coordinates of the four α particles ($i = 1, \ldots, 4$). The algebra of $U(10)$ is constructed by introducing three vector bosons b_ρ, b_λ, and b_η together with an auxiliary scalar boson s. The bilinear products of creation and annihilation operators generate the algebra $U(10)$

$$b^\dagger_{\rho,m}, b^\dagger_{\lambda,m}, b^\dagger_{\eta,m}, s^\dagger \equiv c^\dagger_\alpha \qquad (m = 0, \pm 1),$$
$$\mathcal{G}: G_{\alpha\beta} = c^\dagger_\alpha c_\beta \qquad (\alpha, \beta = 1, \ldots, 10).$$

The creation and annihilation operators for vector bosons ($b^\dagger_{\rho,m}$, $b^\dagger_{\lambda,m}$, $b^\dagger_{\eta,m}$ and $b_{\rho,m}$, $b_{\lambda,m}$, $b_{\eta,m}$) represent the second quantized form of the Jacobi coordinates and their canonically conjugate momenta, whereas the auxiliary scalar boson is introduced in order to construct the spectrum generating algebra. The energy levels can be obtained by diagonalizing the Hamiltonian H. In this Letter, we consider clusters composed of four identical particles (4α), for which H must be invariant under the permutation group S_4. The most general one- and two-body Hamiltonian that describes the relative motion of four identical particles, is a scalar under S_4, is rotationally invariant, and conserves parity as well as the total number of bosons is given by [13,14]

$$
\begin{aligned}
H = {} & \epsilon_0 s^\dagger \tilde{s} - \epsilon_1 (b_\rho^\dagger \cdot \tilde{b}_\rho + b_\lambda^\dagger \cdot \tilde{b}_\lambda + b_\eta^\dagger \cdot \tilde{b}_\eta) + u_0 s^\dagger s^\dagger \tilde{s}\,\tilde{s} - u_1 s^\dagger (b_\rho^\dagger \cdot \tilde{b}_\rho + b_\lambda^\dagger \cdot \tilde{b}_\lambda + b_\eta^\dagger \cdot \tilde{b}_\eta)\tilde{s} \\
& + v_0[(b_\rho^\dagger \cdot b_\rho^\dagger + b_\lambda^\dagger \cdot b_\lambda^\dagger + b_\eta^\dagger \cdot b_\eta^\dagger)\tilde{s}\,\tilde{s} + \text{H.c.}] + \sum_{L=0,2} a_L [[2 b_\rho^\dagger b_\eta^\dagger + 2\sqrt{2} b_\rho^\dagger b_\lambda^\dagger]^{(L)} \cdot [\text{H.c.}]^{(L)} \\
& + [2 b_\lambda^\dagger b_\eta^\dagger + \sqrt{2}(b_\rho^\dagger b_\rho^\dagger - b_\lambda^\dagger b_\lambda^\dagger)]^{(L)} \cdot [\text{H.c.}]^{(L)} + [b_\rho^\dagger b_\rho^\dagger + b_\lambda^\dagger b_\lambda^\dagger - 2 b_\eta^\dagger b_\eta^\dagger]^{(L)} \cdot [\text{H.c.}]^{(L)}] \\
& + \sum_{L=0,2} c_L [[-2\sqrt{2} b_\rho^\dagger b_\eta^\dagger + 2 b_\rho^\dagger b_\lambda^\dagger]^{(L)} \cdot [\text{H.c.}]^{(L)} + [-2\sqrt{2} b_\lambda^\dagger b_\eta^\dagger + (b_\rho^\dagger b_\rho^\dagger - b_\lambda^\dagger b_\lambda^\dagger)]^{(L)} \cdot [\text{H.c.}]^{(L)}] \\
& + c_1 [(b_\rho^\dagger b_\lambda^\dagger)^{(1)} \cdot (\tilde{b}_\lambda \tilde{b}_\rho)^{(1)} + (b_\lambda^\dagger b_\eta^\dagger)^{(1)} \cdot (\tilde{b}_\eta \tilde{b}_\lambda)^{(1)} + (b_\eta^\dagger b_\rho^\dagger)^{(1)} \cdot (\tilde{b}_\rho \tilde{b}_\eta)^{(1)}] \\
& + \sum_{L=0,2} d_L (b_\rho^\dagger b_\rho^\dagger + b_\lambda^\dagger b_\lambda^\dagger + b_\eta^\dagger b_\eta^\dagger)^{(L)} \cdot (\text{H.c.})^{(L)}, \qquad (1)
\end{aligned}
$$

with $\tilde{b}_{km} = (-1)^{1-m} b_{k-m}$ ($k = \rho,\ \lambda,\ \eta$) and $\tilde{s} = s$. The coefficients ϵ_0, ϵ_1, u_0, u_1, v_0, a_0, a_2, c_0, c_2, c_1, d_0, and d_2 parametrize the interactions. The Hamiltonian H is diagonalized within the space of the totally symmetric representation $[N]$ of $U(10)$.

Associated with the Hamiltonian H are transition operators T. Electromagnetic transition rates and form factors can all be calculated by considering the matrix elements of the operator

$$
T = e^{-iq\beta D_{\eta,z}/X_D}, \qquad D_{\eta,m} = (b_\eta^\dagger \times \tilde{s} - s^\dagger \times \tilde{b}_\eta)_m^{(1)}, \qquad (2)
$$

which is the algebraic image of the operator $\exp(iqr_{4,z})$ obtained from the full operator $\sum_{i=1}^{4} \exp(i\vec{q} \cdot \vec{r}_i)$ by choosing the momentum transfer $\vec{q}$ in the z direction taken perpendicular to the base triangle in the direction of the fourth α particle and considering all particles to be identical (the coefficient X_D is a normalization factor).

The Hamiltonian of Eq. (1) with an appropriate choice of parameters can describe any dynamics of four-particle systems. In two cases, corresponding to the dynamic symmetries $U(10) \supset U(9)$ (harmonic oscillator) and $U(10) \supset SO(10)$ (deformed oscillator), the eigenvalues of the Hamiltonian H of Eq. (1) can be obtained analytically. Here, we discuss another situation, namely, that of four particles at the vertices of a tetrahedron with $\mathcal{T}_d$ symmetry. The spectrum of a tetrahedral configuration can be obtained from the Hamiltonian of Eq. (1) by setting some coefficients equal to zero and taking specific linear combinations of others [13,14]

$$
\begin{aligned}
H = {} & \xi_1 (R^2 s^\dagger s^\dagger - b_\rho^\dagger \cdot b_\rho^\dagger - b_\lambda^\dagger \cdot b_\lambda^\dagger - b_\eta^\dagger \cdot b_\eta^\dagger)(\text{H.c.}) + \xi_2 [(-2\sqrt{2} b_\rho^\dagger \cdot b_\eta^\dagger + 2 b_\rho^\dagger \cdot b_\lambda^\dagger)(\text{H.c.}) \\
& + (-2\sqrt{2} b_\lambda^\dagger \cdot b_\eta^\dagger + (b_\rho^\dagger \cdot b_\rho^\dagger - b_\lambda^\dagger \cdot b_\lambda^\dagger))(\text{H.c.})] + \xi_3 [(2 b_\rho^\dagger \cdot b_\eta^\dagger + 2\sqrt{2} b_\rho^\dagger \cdot b_\lambda^\dagger)(\text{H.c.}) \\
& + (2 b_\lambda^\dagger \cdot b_\eta^\dagger + \sqrt{2}(b_\rho^\dagger \cdot b_\rho^\dagger - b_\lambda^\dagger \cdot b_\lambda^\dagger))(\text{H.c.}) + (b_\rho^\dagger \cdot b_\rho^\dagger + b_\lambda^\dagger \cdot b_\lambda^\dagger - 2 b_\eta^\dagger \cdot b_\eta^\dagger)(\text{H.c.})] + \kappa_1 \vec{L} \cdot \vec{L} + \kappa_2 (\vec{L} \cdot \vec{L} - \vec{I} \cdot \vec{I})^2. \qquad (3)
\end{aligned}
$$

Here, $\vec{L}$ denotes the angular momentum in coordinate space (x, y, z) and $\vec{I}$ the angular momentum in the so-called "index" space ρ, λ, η.

The eigenvalues of H of Eq. (3), given in terms of five parameters ξ_1, ξ_2, ξ_3, κ_1, κ_2 and the rigidity parameter R^2, cannot be obtained analytically. However, an approximate energy formula can be obtained by semiclassical methods [$N \to \infty$ in $U(10)$]. A tetrahedral configuration has three vibrational modes v_1, v_2, and v_3 labeled by their $\mathcal{T}_d$ symmetry. The vibration v_1 is the symmetric stretching (breathing mode) with A symmetry. The vibration $v_2 = v_{2a} + v_{2b}$ is the doubly degenerate vibration with E symmetry and a, b components. The vibration $v_3 = v_{3a} + v_{3b} + v_{3c}$ is the triply degenerate vibration with F symmetry and a, b, c components. Since the tetrahedral group $\mathcal{T}_d$ is isomorphic to the permutation group S_4, the vibrations can also be labeled by representations of S_4: $[4] \sim A$, $[22] \sim E$, $[31] \sim F$. The vibrational spectrum is

$$
E_{\text{vib}} = \omega_1 \left(v_1 + \frac{1}{2}\right) + \omega_2 (v_2 + 1) + \omega_3 \left(v_3 + \frac{3}{2}\right), \qquad (4)
$$

with frequencies

$$
\omega_1 = 4NR^2 \xi_1, \qquad \omega_2 = \frac{8NR^2}{1+R^2} \xi_2, \qquad \omega_3 = \frac{8NR^2}{1+R^2} \xi_3. \qquad (5)
$$

For rigid configurations, $R^2 = 1$ and $\omega_i = 4N\xi_i$ (with $i = 1,\ 2,\ 3$). The rotational states built on top of each vibration have angular momenta and parities determined by the invariance of the Hamiltonian under S_4; i.e., all states must be symmetric under S_4. As a consequence, states with A symmetry have angular momentum and parity $L^P = 0^+$, 3^-, 4^+, $6^\pm$, …, while states with E symmetry have $L^P = 2^\pm$, $4^\pm$, $5^\pm$, $6^\pm$, …, and states with F symmetry have $L^P = 1^-$, 2^+, $3^\pm$, $4^\pm$, $5^{-\pm}$, $6^{+\pm}$, …. Note the unusual composition of the rotational band built on the ground state

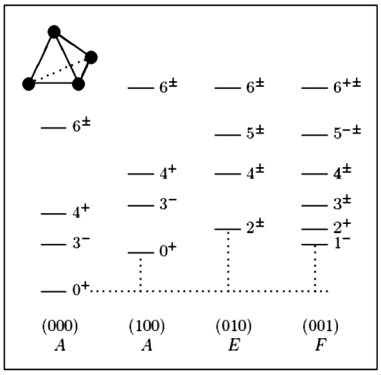

FIG. 1. Schematic spectrum of a spherical top with tetrahedral symmetry and $\omega_1 = \omega_2 = \omega_3$. The rotational bands are labeled by (v_1, v_2, v_3) (bottom). All states are symmetric under S_4.

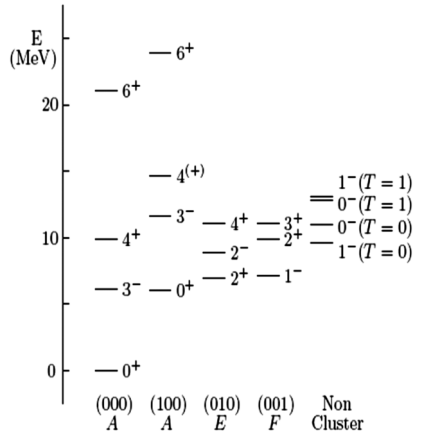

FIG. 2. The observed spectrum of ^{16}O [17]. The levels are organized in columns corresponding to the ground-state band and the three vibrational bands with A, E, and F symmetry of a spherical top with tetrahedral symmetry. The last column shows the lowest noncluster levels.

(A symmetry). This angular momentum content is in agreement with that observed in molecules with $\mathcal{T}_d$ symmetry (see p. 450 of Ref. [15]). This content has also been derived in Ref. [7] for applications to nuclei. The rotational spectrum depends on L and I and on the parameters κ_1 and κ_2 in Eq. (3). However, for the excitations of a rigid spherical top, $L = I$, the last term in Eq. (3) does not contribute, and the rotational energies are given by $E_{\rm rot} = \kappa_1 L(L+1)$. The combined rotation-vibration spectrum of a tetrahedral cluster is shown in Fig. 1.

The matrix elements of the electromagnetic transition operator T and form factors in the ACM are the representation (Wigner) matrix elements of $U(10)$. We have derived closed forms of these in the $U(9)$ and $SO(10)$ dynamic symmetries and in the large N limit for the spherical top with tetrahedral symmetry. This constitutes an important new result of the ACM. In the spherical top case discussed here, the form factors for transitions along the ground-state band $(0,0,0)A$ are given by spherical Bessel functions, $F_L(0^+ \to L^P; q) = c_L j_L(q\beta)$. The coefficients c_L for the first few states are $c_0^2 = 1$, $c_3^2 = 35/9$, $c_4^2 = 7/3$, and $c_6^2 = 416/81$ for $L^P = 0^+$, 3^-, 4^+, and 6^+, respectively. The transition probabilities $B(EL)$ can be extracted from the form factors in the long wavelength limit

$$B(EL; 0 \to L) = \left(\frac{Ze\beta^L}{4}\right)^2 \frac{2L+1}{4\pi}\left[4 + 12P_L\left(-\frac{1}{3}\right)\right]. \tag{6}$$

The form factors and $B(EL)$ values only depend on the parameter β, the distance of each α particle from the center of the tetrahedral configuration, and on the $\mathcal{T}_d$ symmetry that gives the coefficients c_L. By extracting the value of β from the elastic form factor measured in electron scattering, one can, thus, make a model independent test of the symmetry.

Whereas L is an exact symmetry of H, I is not. If $L \neq I$, perturbations must be added. The algebraic model allows one to study these perturbations quantitatively by diagonalizing the Hamiltonian H of Eq. (3) in an appropriate basis. A convenient basis to construct states with good permutation symmetry S_4 is the nine-dimensional harmonic oscillator basis [16] corresponding to the reduction $U(10) \supset U(9) \supset U(3) \otimes U(3) \otimes U(3)$. We have constructed a set of computer programs to calculate energies and electromagnetic transition rates in this basis.

Our derivation of the spectrum of clusters with $\mathcal{T}_d$ symmetry can be used to study cluster states in ^{16}O. The observed experimental spectrum of ^{16}O is shown in Fig. 2. It appears that a rotational ground-state band with angular momenta $L^P = 0^+$, 3^-, 4^+, 6^+ has been observed with moment of inertia such that $\kappa_1 = 0.511$ MeV. It appears also that all three vibrations A, E, and F, have been observed with comparable energies, $\sim$6 MeV, as one would expect from Eq. (4) if $\xi_1 = \xi_2 = \xi_3$. A rotational band with 0^+, 3^-, 4^+, 6^+ also appears to have been observed for the A vibration (1,0,0) (breathing mode). This band is similar in nature to the band built on the Hoyle state in ^{12}C and recently observed [2–4]. It has a moment of inertia such that $E = 0.463L(L+1)$ MeV. The moment of inertia of the A vibration is greater than that of the ground state due to its nature (breathing vibration). The situation is summarized in Fig. 3. The observed spectrum has perturbations. The most notable perturbation is the splitting of the $2^{\pm}$ states of the E vibration. This cannot be simply described by the formula $E \propto L(L+1)$ and requires a diagonalization of the full Hamiltonian.

Having identified the cluster states, one can then test the $\mathcal{T}_d$ symmetry by means of the electromagnetic form factors and $B(EL)$ values. We extracted the value of β from the first minimum in the elastic form factor [18], obtaining $\beta = 2.0$ fm. Table I shows the results for the $B(EL)$ values. The $\mathcal{T}_d$ symmetry appears to be unbroken in the

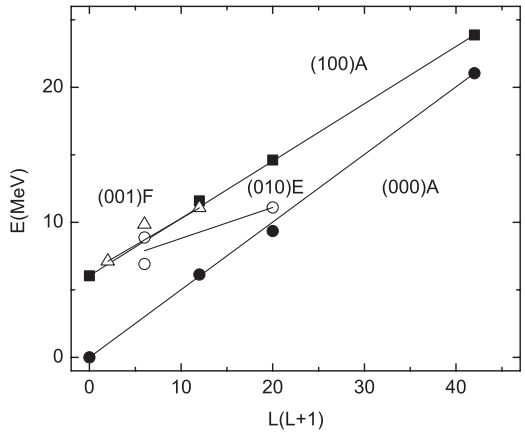

FIG. 3. The excitation energies of cluster states in ^{16}O plotted as a function of $L(L+1)$: closed circles for the ground-state band, closed squares for the A vibration, open circles for the E vibration, and open triangles for the F vibration.

ground-state band of ^{16}O. We also investigated the electromagnetic decays of the vibrational bands $(1,0,0)A$, $(0,1,0)E$, and $(1,0,0)F$. For these bands, the $\mathcal{T}_d$ symmetry appears to be broken and, in addition, they decay mostly by $E2$ quadrupole transitions. For $E2$ transitions, the simple analytic formula of Eq. (6) does not apply, since the $E2$ operator is not in the representation A of $\mathcal{T}_d$ as the $E3$, $E4$, and $E6$ operators and, hence, can connect different representations. A full account of these transitions will be given in a forthcoming longer publication [19].

Cluster states represent only a portion of the full spectrum of states. They are obtained by assuming that the α particles have no internal excitation. At energies of the order of the shell gap, ~16 MeV in ^{16}O, one expects to have noncluster states and, thus, the spectrum to be composed of cluster states immersed into a bath of noncluster states. Assigning states to cluster or noncluster above this energy is a difficult task. We note, however, that the tetrahedral structure in Fig. 1 has *no* 0^- state and only one 1^- state in the F vibration. Thus, 0^- states are clearly noncluster states. Also, with α particles, one cannot form $T=1$ states. These states are obviously noncluster. In Fig. 2, we have assigned the states $L^P=1^-, 0^-(T=0)$ at $E=9.585$ and 10.957 MeV and $L^P=0^-, 1^-(T=1)$ at $E=12.796$ and 13.090 MeV, as the shell-model configuration $1p_{1/2}^{-1}2s_{1/2}$. The shell-model states $1p_{1/2}^{-1}1d_{5/2}$ with $L^P=2^-, 3^-$ and $T=0$ and $T=1$ can also be easily identified, but they are not shown in Fig. 2 to not overcrowd the figure. For the same reason, we do not show in Fig. 2 other states with $L^P=4^\pm, 5^-, 6^\pm,\ldots$, which can be assigned to cluster configurations.

An important question is the shell-model description of cluster states. It was suggested long ago [20,21] that the state at 6.049 MeV is $4p-4h$, while the state at 7.116 MeV is $5p-5h$. In view of the recent developments of large-scale shell-model calculations and of the no-core shell model it would be interesting to study once more the shell-model description of the states in Fig. 2.

Very recently, also, an *ab initio* lattice calculation of the spectrum and structure of ^{16}O was reported [22]. This calculation confirms the tetrahedral structure of the ground state of ^{16}O in agreement with our findings. For the excited states, 0_2^+ and 2_1^+ instead, a square configuration is suggested. This would imply a large breaking of the $\mathcal{T}_d$ symmetry for the vibrations in Fig. 2. Although we expect the $\mathcal{T}_d$ symmetry to be broken for the vibrational states due to the near degeneracy of them $\xi_1=\xi_2=\xi_3$, i.e., even a small breaking term in H may cause a large mixing, we nonetheless feel at this stage that our interpretation of the excited states of ^{16}O as vibrations provides a good starting point for further studies. Algebraic methods are quite general, and as shown in Ref. [23], they can accommodate all sorts of configurations of four particles, including configurations with $\mathcal{T}_d$, $\mathcal{D}_{3h}$, and $\mathcal{D}_{4h}$ (square) symmetry. In connection with tetrahedral configurations in nuclei, we mention here also the work of Ref. [24] in light nuclei and Ref. [25] in heavy nuclei for which, however, there is no experimental confirmation.

In conclusion, we have introduced an algebraic model capable of describing the full dynamics of four-body clusters. Within this model, we have rederived the spectrum of a spherical top with tetrahedral symmetry and confirmed the evidence for the occurrence of this symmetry in the low-lying spectrum of ^{16}O presented long ago by Kameny [7] and Robson [10]. An analysis of the $B(EL)$ values along the ground-state band provides even stronger evidence for $\mathcal{T}_d$ symmetry than the energies. Another crucial aspect is the development of the $U(10)$ ACM for four-body clusters that allows a detailed description of energies, electromagnetic transition rates, form factors, and $B(EL)$ values. We hope that the results in this Letter will stimulate further

TABLE I. Comparison of theoretical and experimental $B(EL)$ values in $e^2\,\mathrm{fm}^{2L}$ and E_γ values in keV, along the ground-state band. The theoretical $B(EL)$ values are obtained from Eq. (6), and the E_γ values are obtained from $E=0.511L(L+1)$ MeV. The experimental values are taken from Ref. [17].

$B(EL;L^P\to 0^+)$	Theoretical	Experimental	$E_\gamma(L^P)$	Theoretical	Experimental
$B(E3;3_1^-\to 0_1^+)$	181	205 ± 10	$E_\gamma(3_1^-)$	6132	6130
$B(E4;4_1^+\to 0_1^+)$	338	378 ± 133	$E_\gamma(4_1^+)$	10220	10356
$B(E6;6_1^+\to 0_1^+)$	8245		$E_\gamma(6_1^+)$	21 462	21 052

experimental work on the structure of ^{16}O. Finally, the results presented here in conjunction with those in ^{12}C emphasize the occurrence of α-cluster states in light nuclei.

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