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Shape isomers and molecular states in ³²S

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The sequences of states found in a microscopically derived ${}^{16}O_{-}{}^{16}O$ potential are identified by energies and quadrupole moments as candidates for shape isomeric and molecular bands in ${}^{32}S$. The B(E2) transitions within and between the bands and the capture cross sections into shape isomers and molecular states are calculated.

[NUCLEAR REACTIONS ³²S; calculated shape isomeric and molecular bands; microscopically derived potential model; electromagnetic transitions.

Long-lived, highly deformed states in light nuclei like 32 S have been predicted in several theoretical approaches.¹⁻⁴ Shell model and constrained Hartree-Fock calculations give evidence for the existence of so-called shape isomeric states with high clustering found in a second minimum in the potential surfaces.^{1,2} Microscopic³ as well as phenomenological⁴ models predict long-lived quasibound states found in the pocket of the heavy-ion potential. These states, often referred to as molecular states, are assumed to be responsible for the intermediate resonant structure found in excitation functions of several heavy-ion systems.⁵

Although predicted on strong and diverse theoretical grounds, the existence of shape isomers and molecular states in light nuclei has not yet been confirmed experimentally. The experimental search for long-lived deformed states in light nuclei is much more difficult than for fission isomers in the actinide region, since these states cannot be detected by the conventional isomer spectroscopy due to much stronger background. It is therefore believed⁶ that an experimental identification of shape isomeric or molecular states in light nuclei has to rely on some conjectured level sequences whose band properties agree with the picture of deformed states. Obviously the experimental searches are aided by theoretical estimates of the properties of these deformed states, such as energies, quadrupole deformations, and B(E2) transition strengths.

In the present paper we report theoretical predictions for the properties of shape isomeric and molecular states in ³²S. This calculation is based on the local ¹⁶O-¹⁶O potential microscopically derived from the exact potential kernels of the generator coordinate method.⁷ Consequently, the study satisfies conditions which are indispensable for a meaningful investigation of long-lived, deformed states: antisymmetrization and angular momentum projection are taken into account exactly. Our calculation differs from previous studies in that it also allows us to study excited deformed states and nonresonant states in an easy and microscopically consistent way. In the present case of ³²S, our Hamiltonian predicts two sequences of long-lived deformed states, which in accordance to other theoretical approaches can be envisioned as shape isomeric and molecular states, respectively, and for which there might be some experimental support. This allows us to calculate the electromagnetic transitions within a shape or molecular band as well as the cross sections into shape isomeric and molecular states, both of which might be quite useful for an experimental identification of these states.

In accord with previous studies, we assume in our calculation that the deformed ^{32}S states (angular momentum l) are described by antisymmetrized products

 $\mathscr{A}[\Phi_0^1(\xi_1)\Phi_0^2(\xi_2)g_l(x)].$ (1)

The fragments are described by their harmonic oscillator shell model ground states, while the unknown wave functions $g_I(x)$ are determined by solving the Schrödinger equation of relative motion:

$$\Lambda \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) + \frac{l(l+1)\hbar^2}{2\mu x^2} - E \right] g_l(x) = 0 .$$
(2)

The Pauli projector Λ , which projects off the Pauli forbidden states,^{8,9} is a consequence of the fact that exchange antisymmetrization between the two fragments is considered in Eq. (1). Since the internal degrees of freedom of the fragments are described within the harmonic oscillator shell model, the Pauli forbidden states are known exactly. In principle, Eq. (2) is the exact orthogonalized version of the resonating group, but in practice the potential V(x) is taken as an approximation to the exact potential kernels of the resonating group or the generator coordinate method (see Ref. 9 and references given therein). To retain the microscopic character of our approach as much as possible, the nucleus-nucleus potential in (2) is adopted as the four Gaussian potential of Ref. 7, which is microscopically derived from the exact GCM kernels. The Coulomb part is assumed as the potential of a homogeneously charged sphere with radius 3.8 fm.¹⁰

Let h_l and k_l denote the relative wave function of a ³²S bound state or narrow resonance¹¹ of type (1) as determined by Eq. (2). Then the E2 transition between these states is given by

$$T_{fi} = \langle \Phi_0^1 \Phi_0^2 h_l \mid \mathscr{A}Q \mathscr{A} \mid \Phi_0^1 \Phi_0^2 k_{l'} \rangle , \qquad (3)$$

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where

$$Q = \sum_{i=1}^{32} \frac{e}{2} (1 - \tau_{zi}) x_i^2 Y_2(\hat{x}_i) .$$
(4)

For simplicity we suppress the index *m* throughout this paper. Since states of type (1) are T=0 states, only the isoscalar part of Q (denoted by \hat{Q}) can contribute to (3). Furthermore, \hat{Q} can be factorized into

$$\hat{Q} = Q_{0,1} + Q_{0,2} + Q_{\text{rel}}$$
, (5)

where $Q_{0,1}$ and $Q_{0,2}$ only act on the internal coordinates of fragments 1 and 2, while Q_{rel} is given by

$$Q_{\rm rel} = \mu \frac{e}{2} x^2 Y_2(\hat{x}) ,$$
 (6)

where μ is the reduced mass. Equation (3) can be rewritten as¹²⁻¹⁴

$$\langle \Phi_{0}^{1} \Phi_{0}^{2} h_{l} | \mathscr{A} Q \mathscr{A} | \Phi_{0}^{1} \Phi_{0}^{2} k_{l'} \rangle = \sum_{n,n'} \langle h_{l} | u_{n,l} \rangle \langle u_{n',l'} | k_{l'} \rangle \langle u_{n,l} | Q_{\text{rel}} | u_{n',l'} \rangle \mu_{2N+L} , \qquad (7)$$

with

$$\mu_{2N+L} = \langle \Phi_0^1 \Phi_0^2 u_{N,L} \mid \mathscr{A} \mid \Phi_0^1 \Phi_0^2 u_{N,L} \rangle$$
(8)

and

$$2N+L=\min(2n+l,2n'+l').$$

The functions $u_{n,l}(x)$ are radial harmonic oscillator wave functions of width $\beta^2 = b^2/\mu$, where b is the oscillator parameter of the internal factors in (1) (b = 1.58 fm). The quantities μ_{2N+L} are known analytically,¹⁵ while the evaluation of the remaining matrix elements in (7) can be performed numerically.

The reduced $B(E2, l' \rightarrow l)$ matrix element between two states is finally given by

$$B(E2, l' \to l) = \frac{1}{(2l'+1)} |T_{fi}|^2.$$
(9)

The radiative E2 capture cross section $\sigma_{I,I'}(E)$ from a scattering state $\mathscr{A} \mid \Phi_0^1 \Phi_0^2 \varphi_{I'}$ at energy E into a bound state or narrow resonance at E_0 is given by

$$\sigma_{l,l'}(E) = \frac{4\pi}{75} \frac{1}{\hbar v_{\text{rel}}} \left[\frac{E - E_0}{\hbar c} \right]^5 \frac{1}{(2l' + 1)} |T_{fi}|^2, \quad (10)$$

where v_{rel} is the relative velocity in the entrance channel.

We first want to show that the microscopically derived ¹⁶O-¹⁶O potential of Ref. 7 makes reasonable predictions

TABLE I. Energies and quadrupole moments of the ³²S shape isomers as predicted by the ¹⁶O-¹⁶O potential of Ref. 7. For comparison we also list the energies E_{exp} of the experimental candidates for the ³²S shape isomers as suggested in Ref. 6. The energies are excitation energies in ³²S. The resulting internal quadrupole moment is $Q_0=2.19$ b.

1	E (MeV)	$\begin{array}{c} Q \\ (e \ \mathrm{fm}^2) \end{array}$	$E_{\rm exp}$ (MeV)
0	8.40		8.51
2	8.90	-62.7	9.06
4	10.31	- 79.5	10.28
6	12.52	- 87.9	
8	15.47	-92.6	
10	18.88	-95.0	

about shape isomers and molecular states in ${}^{32}S$. By solving Eq. (2) with this potential, we find three series of bound or resonance states. The ground state band of the potential has a band head at $E_{\rm c.m.} = -8.14$ MeV (corresponding to an excitation energy of $E^* = 8.40$ MeV in ${}^{32}S$) and a rotational constant of

$$\Delta E/l(l+1) \approx 95$$
 keV.

The members of the ground state band with l < 10 are bound states, for $l \ge 10$ they are narrow resonances. The first excited band is formed of narrow ("molecular") resonances with a band head at $E_{\rm c.m.} = 3.59$ MeV. The third band starts at $E_{\rm c.m.} \approx 10.8$ MeV, close to the Coulomb barrier. Its members are rather broad ("shape") resonances with widths of 1–3 MeV. It should be noted that the ³²S ground state band cannot be described by a cluster ansatz of type (1) and is therefore not included in our calculation.

In Table I we have listed the energies and electric quadrupole moments Q for the lowest band of the potential with $l \leq 10$. These results correspond to a sequence of rotational states with an internal quadrupole moment $Q_0=2.19$ b with deviations of less than 0.5% between the different members of the rotational band. The energies of these states agree to within 100 keV with those of the ³²S states recently suggested as experimental candidates for the ³²S isomeric states.⁶ The present results are also in ex-

TABLE II. Energies and quadrupole moments of the ³²S molecular states as predicted by the ¹⁶O-¹⁶O potential of Ref. 7. The energies are c.m. energies in the ¹⁶O-¹⁶O system. The resulting internal quadrupole moment is $Q_0 = 3.09$ b.

	E	0
l	(MeV)	$(e \ \mathrm{fm}^2)$
0	3.59	
2	4.41	- 88.0
4	5.43	-112.3
6	7.03	-123.9
8	9.09	-130.5
10	11.43	-132.4
12	13.32	- 124.6
14	16.88	-122.5
16	22.72	- 143.4

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TABLE III. Reduced $B(E2, l_i \rightarrow l_f)$ matrix elements for the transitions within the shape isomeric and molecular bands.

		$ B(E2, l_i \rightarrow l_f) \\ (e^2 \text{ fm}^4) $	
l _i	l_f	Shape isomeric	Molecular
2	0	960.4	1855.1
4	2	1361.8	2700.9
6	4	1500.3	2989.5
8	6	1577.7	3131.2
10	8	1607.3	3155.7
12	10		2787.3
14	12		2588.7
16	14		2715.8

cellent agreement with previous calculations; i.e., in a variational study using the α -particle model, Schultheis and Schultheis⁶ predicted a band of shape isomers starting at $E_{\rm c.m.} \approx 7.12$ MeV with an internal quadrupole deformation of $Q_0=2.08$ b, and in a self-consistent heavy-ion potential calculation (although without angular momentum projection), Zint and Mosel² predicted a shape isomeric band starting at an excitation energy of 8–9 MeV and with $Q_0=1.95$ b.

The energies and the quadrupole moments of the first excited (molecular) band are given in Table II. Except for a small antistretching effect in the partial waves l=12 and 14, whose physical significance is unclear, all members of the excited band have the same internal moment $Q_0 = 3.09$ b with deviations of less than 1%. Due to numerical convergence problems the deformations of the broad resonant states cannot be calculated as outlined above. The energies of these states are given in Ref. 16.

TABLE IV. Reduced $B(E2, l_i \rightarrow l_f)$ matrix elements for the transition from the molecular band into the shape isomeric band.

 1.	1.	$B(E2, l_i \rightarrow l_f)$ $(e^2 \text{ fm}^4)$
	• • • •	(c m)
2	0	549.5
0	2	2910.4
2	2	776.6
4	2	788.6
2	4	1411.9
4	4	724.2
6	4	874.7
4	6	1289.3
6	6	739.1
8	6	1009.3
6	8	1276.1
8	8	789.7
10	8	1187.7
8	10	1306.5
10	10	883.8
12	10	1527.0

In a recent study¹⁶ based on the same microscopically derived ¹⁶O-¹⁶O potential, it has been shown that many of the resonant structures observed in inelastic ¹⁶O-¹⁶O reactions can be interpreted as the interaction of molecular and shape resonances in the elastic and the respective inelastic channels. Moreover, the potential of Ref. 7 gives simultaneously a reasonable description of the predicted ³²S shape isomeric states, as well as the ¹⁶O-¹⁶O elastic and inelastic reaction data. Consequently, it seems justified to place some confidence in the capture cross sections and intraband B(E2) values calculated with this potential.

The reduced B(E2) matrix elements for the E2 transition within the shape isomeric and molecular bands are given in Table III, while the B(E2) values for transition from the molecular band to the shape isomers are listed in Table IV. Compared to a single particle Weisskopf unit of ~6.1 e^2 fm⁴, the calculated B(E2) values clearly indicate a strong collective phenomenon. For comparison, the



FIG. 1. Capture cross sections into the molecular states at $E_{c.m.} = 13.32$ MeV $(l = 12^+)$ and 16.88 MeV $(l = 14^+)$.

experimental B(E2) values for the shape isomeric states in ²⁸Si are of the order of tens of Weisskopf units.¹⁷

The measurement of the gamma-particle decay branching ratios is generally believed to be a proper tool for the identification of molecular states. Using the B(E2) values as listed in Table III the γ width of the transition between the l = 14 and 12 states in the first excited band is calculated as $\Gamma_{\gamma} = 1.1$ eV. Assuming a reasonable total width not larger than several hundred keV for these states (a one-channel calculation gives an entrance channel width of less than 1 keV), the predicted strong deformation of these states can in principle be tested with present-day experimental facilities by measuring the gamma-particle decay branching ratios.^{18,19} Unfortunately, there is yet no experimental evidence for a long-lived resonance with l=14 near $E_{\rm c.m.} = 17$ MeV in ³²S. The prediction of ¹⁶O-¹⁶O molecular states might be

tested by measuring the gamma-particle decay branching ratio for one of the long-lived resonances with spins J=8and 10 which have been observed^{20,21} in the range $E_{\rm c.m.} = 15 - 17$ MeV. However, one should consider that these resonances are likely to be due to molecular states in aligned ¹⁶O-¹⁶O inelastic channels excited via a doubleresonance mechanism²² rather than to molecular resonances in the elastic channel. Since similar resonance structure is expected in the elastic and various inelastic ¹⁶O-¹⁶O channels, the experimental detection of molecular states in inelastic channels might be envisioned as an indirect test for the existence of molecular states in the elastic channel. The fact that these narrow structures might arise from resonances in aligned inelastic channels would have strong consequences for a measurement of the gamma-particle decay branching ratio: Assuming an l(l+1) energy dependence within the molecular band, the observed γ energy for an intraband transition in an aligned inelastic channel will be noticeably smaller than for a transition within the elastic band, since the transition in the aligned channel will occur from a molecular state with relative angular momentum l = J - I (*I* is the channel spin of the inelastic channel) rather than from a state with l = J.

In Fig. 1 we have plotted the radiative capture cross sections for the partial waves l-2, l, and l+2 into the molecular states at $E_{\rm c.m.} = 13.32$ MeV ($l=12^+$), and 16.88 MeV ($l=14^+$), as calculated from (10). One clearly sees that the cross sections exhibit structures which can be traced back to resonances in the different partial waves. The broad bumps with a magnitude of about 10 μ b reflect the barrier resonances. The pronounced narrow structures found in the transitions $l \rightarrow l-2$ correspond to the intraband transition of the molecular band; for this transition the cross sections reflect a sign change in the matrix element (3). They may be viewed as consequences of the exact treatment of the Pauli principle, since they vanish if antisymmetrization is switched off.

In Fig. 2 we have plotted the cross sections for the transition into shape isomeric states at $E_{\rm c.m.} = -8.14$ MeV $(l=0^+)$ and $E_{\rm c.m.} = -7.64$ MeV $(l=2^+)$. The cross section always exhibits peaks near those energies at which the incoming partial wave has a broad barrier resonance. Despite the fact that the energies of the photons are $\approx 15-20$ MeV, the cross sections only approach a few μb , since the deformations of the shape isomeric states are quite different from those of the barrier resonances. To detect the head of the ³²S shape isomeric band, a much higher cross section can be expected from a transition between a molecular state and a shape isomeric state, as is



FIG. 2. Capture cross sections into the shape isomeric states at $E_{c.m.} = -8.14$ MeV $(l=0^+)$ and -7.64 MeV $(l=2^+)$.

suggested by the B(E2) matrix elements of Table IV. Unfortunately a direct excitation of molecular states with small *l* values in the elastic ¹⁶O-¹⁶O channel is rather unlikely, since these states are located well below the Coulomb barrier. A possible way out of this dilemma would be to use the experimentally observed narrow resonances at 10–12 MeV (Ref. 23) as doorway states into the shape isomers, since these states have been suggested as molecular states in inelastic ¹⁶O-¹⁶O channels excited in a double resonance mechanism.¹⁶ Another possibility to detect the isomeric states is discussed in Ref. 6, which suggested the α -²⁸Si channel as a proper entrance channel to excite these states.

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