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GROUND STATE NUCLEAR PROPERTIES OF Mo AND Ru ISOTOPES IN SKYRME-HARTREE-FOCK-BOGOLIUBOV METHOD

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Abstract. Ground-state nuclear properties of Mo and Ru isotopes were studied within the Hartree-Fock-Bogoliubov method with SLy4 and SLy5 Skyrme forces. Nuclei which have neutron numbers close to magic number 50 have received much attention because the nuclei are known well deformed and exhibit anomalous behaviour in the isotope shifts. Therefore, a systematic study of even-even Mo and Ru isotopes was carried out. Almost all ground-state properties which include binding energy per nucleon, quadrupole deformation, nuclear radii, two-neutron separation energy and shape-coexistence for axially deformed Mo and Ru isotopes were analyzed. The results were compared with available experimental data and predictions of some nuclear models (Finite Range

Liquid-Drop Model (FRDM), Extended Thomas Fermi Model with Strutinski Integral (ETF-SI) and Relativistic Mean Field (RMF) Theory) and discussed in detail. The results show that the HFB method with SLy4 and SLy5 Skyrme forces is capable of describing of isotopic chain of even-even Mo and Ru nuclei.

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Keywords
Hartree-Fock-Bogoliubov method, even-even Mo and Ru nuclei, binding energy, deformations

INTRODUCTION

Nuclei which have neutron numbers close to magic number 50 exhibit many interesting nuclear properties such as anomalous behavior in the isotope shifts and large transformations of shapes. Therefore, these nuclei are attractive to study both experimentally and theoretically. It has been known for a long time that most nuclei near magic numbers are deformed and most of them can be described by axially deformations. Ground-state properties of Kr, Sr, Zr, Mo and other nuclei which are near the region of these nuclei were investigated with various microscopic models [1-10]. In the present work, some ground-state properties of axially deformed even-even Mo and Ru isotopes using HFB (Hartree-Fock-Bogoliubov) method with SLy4 and SLy5 Skyrme forces were analyzed.

One of the main aims of researches in nuclear physics is to describe the ground-state properties of all nuclei in the periodic table with one nuclear model. Unfortunately, due to lack of understanding in strong interaction and numerical difficulties in handling nuclear many-body problems, so far all microscopic descriptions are only possible on a phenomenological ground [5]. One of the most important phenomenological approaches widely used in nuclear structure calculations is the Skyrme HFB method. The HFB theory unifies both Hartree-Fock method and BCS theory. In this theory, many properties of nuclei can be described in terms of a model of independent particles moving in an average potential whose space dependence closely follows the matter distribution. In the presence of unfilled shells, additional correlations between these particles are founded.

In standard HFB formalism, the many-body Hamiltonian of a system of fermions in occupation number representation has the form

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c_{n_1} c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c_{n_1} c_{n_2} c_{n_4} c_{n_3}, \tag{1}$$

where $\bar{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle$ is the anti-symmetrized matrix element of the two-body effective *N*-*N* interaction. In the Hartree-Fock-Bogoliubov method, the ground-state wave function is defined as the quasi-particle vacuum where the quasi-particle operators (α, α) are connected to the general linear transformation from particle operators via the linear Bogoliubov transformation:

$$\alpha_k = \sum_n (U^*_{nk} c_n + V^*_{nk} c_n), \qquad \alpha_k = \sum_n (V_{nk} c_n + U_{nk} c_n). \tag{2}$$

The basic building blocks of the theory are the density matrix and the pairing tensor. In terms of the normal ρ and pairing κ one-body density matrices, the expectation value of the Hamiltonian (1) could be expressed as an energy functional

$$E[\rho, k] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \mathrm{Tr}\left[\left(e + \tfrac{1}{2}\Gamma\right)\rho\right] - \tfrac{1}{2}\mathrm{Tr}[\Delta\kappa^*] \,, \tag{3}$$

where

$$\Gamma_{n_1 n_3} = \sum_{n_2 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \rho_{n_4 n_2} \,, \qquad \Delta_{n_1 n_2} = \tfrac{1}{2} \sum_{n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4} \,, \tag{4}$$

Variation of energy (6) with respect to normal ρ and pairing κ density results in the HFB equations:

$$\begin{pmatrix} e + \Gamma - \lambda & \Delta \\ -\Delta^* & -(e + \Gamma)^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}, \tag{5}$$

where Δ and λ denote the pairing potential and Lagrange multiplier introduced to fix the correct average particle number, respectively. Modern energy functional (3) contains terms that cannot be simply related to some prescribed effective interaction [14]. For Skyrme forces, the HFB energy (3) has the form of local energy density functional,

$$\mathrm{E}[\rho, \tilde{\rho}] = \int \mathrm{d}^3\, \mathbf{r} \mathcal{H}(\mathbf{r}) \,, \tag{6}$$

where $\mathcal{H}(\boldsymbol{r}) = H(\boldsymbol{r}) + \tilde{H}(\boldsymbol{r})$ is the sum of the mean field and pairing energy densities. Variation of the energy (6) with respect to ρ and $\tilde{\rho}$ of results in Skyrme HFB equations:

$$\sum_{\sigma'} \begin{pmatrix} h(\boldsymbol{r}, \sigma, \sigma') & \tilde{h}(\boldsymbol{r}, \sigma, \sigma') \\ \tilde{h}(\boldsymbol{r}, \sigma, \sigma') & -h(\boldsymbol{r}, \sigma, \sigma') \end{pmatrix} \begin{pmatrix} U(E, \boldsymbol{r}\sigma') \\ V(E, \boldsymbol{r}\sigma') \end{pmatrix} = \begin{pmatrix} E + \lambda & 0 \\ 0 & E - \lambda \end{pmatrix} \begin{pmatrix} U(E, \boldsymbol{r}\sigma') \\ V(E, \boldsymbol{r}\sigma') \end{pmatrix}$$

(7)

where λ is chemical potential. Local fields $h(\boldsymbol{r}, \sigma, \sigma')$ and $\tilde{h}(\boldsymbol{r}, \sigma, \sigma')$ can be calculated in the coordinate space. Details can be found in Ref. [11-13].

DETAILS OF CALCULATIONS

In this study, HFB equations were solved for axially deformed even-even Mo and Ru isotopes using a computer code called HFBTHO written by Stoitsov et al. [13]. In this code HFB equations are solved by expanding quasi-particle wave functions on a finite basis. Because Eq. (7) reduces to a set of radial differential equations, the best solutions of HFB equations are in the coordinate space for spherical nuclei. However, the solution of a deformed HFB equation in coordinate space yields various difficulties and is time-consuming task. Therefore, Stoitsov et al. used the method proposed by

Vautherin [15] to adapt their code used in present study for shorter solution time. In this code the mean field and the pairing field via Hartree-Fock theory with added Lipkin-Nogami pairing are treated separately.

In this work, the oscillator parameter b_0 was chosen as $b_0 = \sqrt{2(\hbar^2/2m)/(49.2\,A^{-1/3})}$ and the basis deformation (β_0) was determined as 0.3 for all calculations. The molybdenum (Mo) and ruthenium (Ru) nuclei considered here are even-even and open-shell nuclei both in protons and neutrons (except N = 50). Pairing and particle number projection were included. The number of oscillator shells taken into account was 20 for fermionic wave functions. There are a number of parameters sets of the Skyrme forces for prediction of the nuclear ground-state properties [16-18]. We used the SLy4 parametrization (not include tensor term) which is widely used in nuclear structure calculations. Also the SLy5 parametrization includes tensor term which is related with the expression of the two-body interaction was used for comparison. Details can be found in Ref. [18]. Sly4 and SLy5 parameters sets used in this study are shown in Table 1.

Table 1: SLy4 and Sly5 parameters sets

Parameter	SLy4	SLy5
t_0(MeV fm^3)	-2488.9	-2484.88
t_1(MeV fm^5)	486.82	462.18
t_2(MeV fm^5)	-546.4	-448.61
t_3(MeV fm^4)	13777	13673
x_0	0.834	0.825
x_1	-0.3440	-0.465
x_2	-1.0	-1.0
x_3	1.354	1.355
W_0(MeV fm^5)	123	126
σ	1/6	1/6

RESULTS AND DISCUSSION

The Skyrme HFB calculations for two isotopic chains in medium heavy region were performed in this study. Isotopes of Mo (Z = 42) and Ru (Z = 44) were considered here. The nuclei in these chains are known to be well deformed, and several shape transitions along these isotopic chains are expected. In the present work, the HFB equations for an axially deformed prolate configuration were solved. Also, for discussion of shape-coexistence these equations for oblate configuration were solved.

In Fig. 1, the calculated binding energies per nucleon (*BE/A*) of Mo and Ru isotopes in both SLy4 and SLy5 parametrizations are shown together with the predictions of Relativistic Mean Field (RMF) Theory [19] and experimental values [20]. In this study, very good convergences of the numerical calculations for the binding energies of Mo and Ru nuclei in both SLy4 and SLy5 Skyrme forces were obtained except ^{90}Ru nuclei in SLy5 parametrization. Therefore the result of the *BE/A* of

^{90}Ru in SLy5 parametrization are not shown in Fig. 1. As can be seen in Fig. 1, the calculated *BE/A* for Mo and Ru isotopes in the HFB theory and RMF theory are in good agreement with the empirical data for Mo and Ru isotopic chains. The minimums in the *BE/A* were observed at the magic neutron number *N* = 50 in the HFB method with SLy4 and SLy5 Skyrme forces as well as the predictions of RMF theory with NL3 Lagrangian parameters set for both of the isotopic chains. The *BE/A* for Mo and Ru isotopes in SLy4 and SLy5 parametrizations were well produced by our calculations. The approximately maximal errors per particle are 0.04 MeV and 0.09 MeV for Mo and Ru isotopes, respectively.

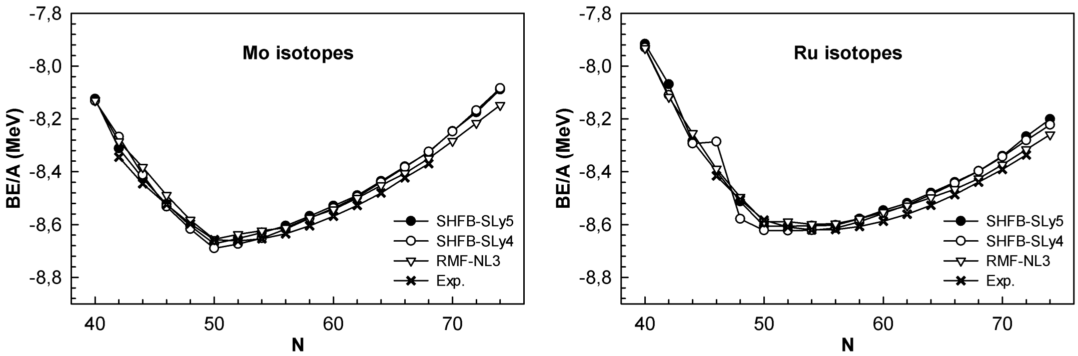

Figure 1: The calculated binding energies per particle for even-even Mo and Ru isotopes in SLy4 and SLy5 parametrizations as a function of neutron number *N*.

Fig. 2 shows the neutron and charge radii of Mo and Ru isotopes obtained in our calculations. The neutron radii show an increase trend with neutron number for both Mo and Ru isotopes. Adding further neutrons, the charge radii of nuclei which are heavier than the closed neutron shell starts increase. Although a king about magic neutron number *N* = 50 were expected in radii curves of Mo and Ru isotopic chains, the neutron radii for these isotopic chains showed a king at four and six neutrons below the closed neutron shell (*N* = 50), respectively. In literature, the same behaviour in isotopic chain of Gd nuclei for *N* = 82 magic number can be seen in Ref. [21]. This behaviour of the neutron radii of Mo and Ru nuclei can be put in perspective.

We obtained the quadrupole moments of Mo and Ru nuclei from the solution of axially deformed HFB equations. Predictions of quadrupole moments of some Mo and Ru isotopes in SLy4 Skyrme force are shown in Table 2. The calculated quadrupole deformation parameters β_2 for these nuclei are shown in Fig. 3. Also, predictions of deformation parameters β_2 of Relativistic Mean Field (RMF) theory with NL3 parameters set [19], Extended Thomas Fermi Model with Strutinski Integral (ETF-SI) method [22], Finite Range Liquid-Drop Model (FRDM) [23] and experimental results [24] are shown in Fig. 3 for comparison. It must be stressed that Fig. 3 does not indicate the sign of the quadrupole deformation parameters β_2. As can be seen in Fig. 3, the calculated β_2 values for Mo and Ru isotopes show a minima at the magic neutron number *N* = 50. This situation were expected because almost all nuclei with $N = 50$ are spherical. The predictions of β_2 in HFB method together with those of RMF, ETF-SI and FRDM were showed small differences from available experimental values. As seen in Fig. 3, for neutron numbers higher than $N = 50$, the prolate deformations increase and then saturate at a value which closes to $\beta_2 = 0.35$ and $\beta_2 = 0.30$ for Mo and Ru isotopes, respectively.

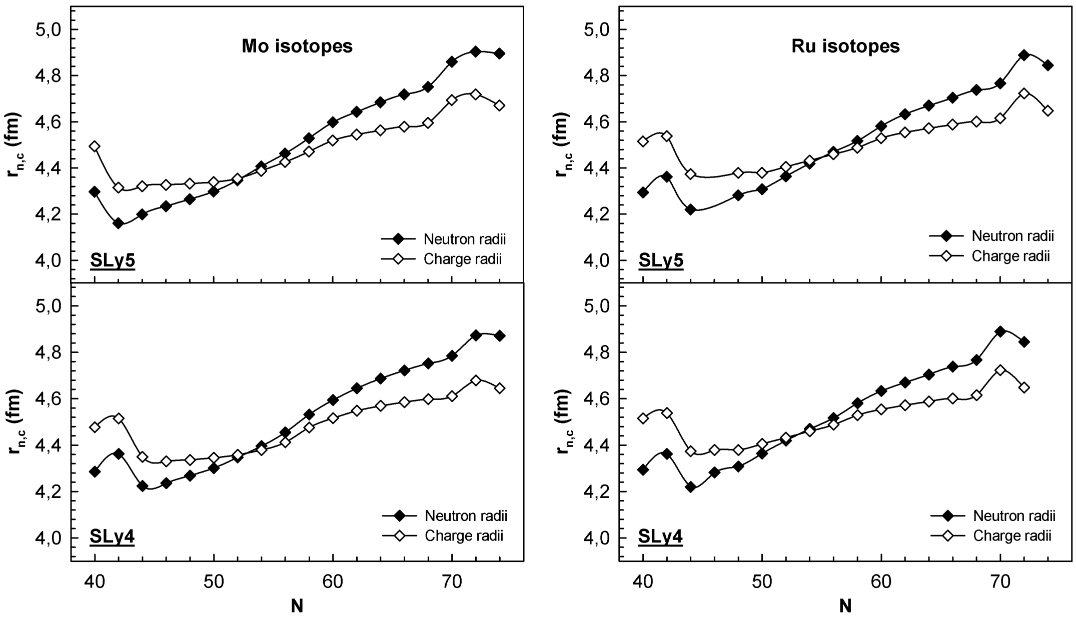

Figure 2: The calculated neutron and charge radii of even-even Mo and Ru isotopes in SLy4 and SLy5 Skyrme forces.

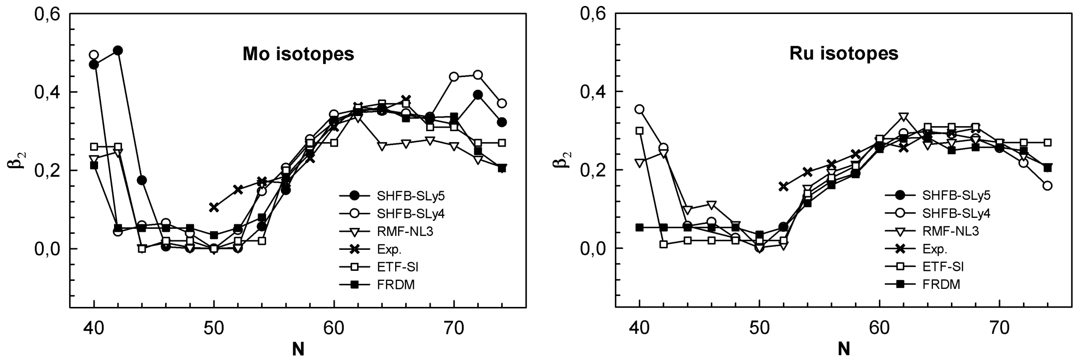

Figure 3: The calculated quadrupole deformation parameter (β_2) for Mo and Ru isotopes in SLy4 and

SLy5 parametrizations as function of neutron number *N*.

In Fig. 4, prolate-oblate shape coexistences of neutron-rich Mo and Ru isotopes obtained using calculated *BE/A* differences between prolate shape configuration and oblate one for the both Skyrme parametrizations are shown as a function of mass number *A*. As can be seen in Fig. 4, Mo and Ru isotopes exhibited a second minimum beside lowest minimum. This implies shape coexistence. The prolate results were a few hundred keV lower in energy than the oblate one in both Mo and Ru nuclei. Also, curves in Fig. 4 shows that results of the SLy4 and SLy5 Skyrme forces are consistent with each other.

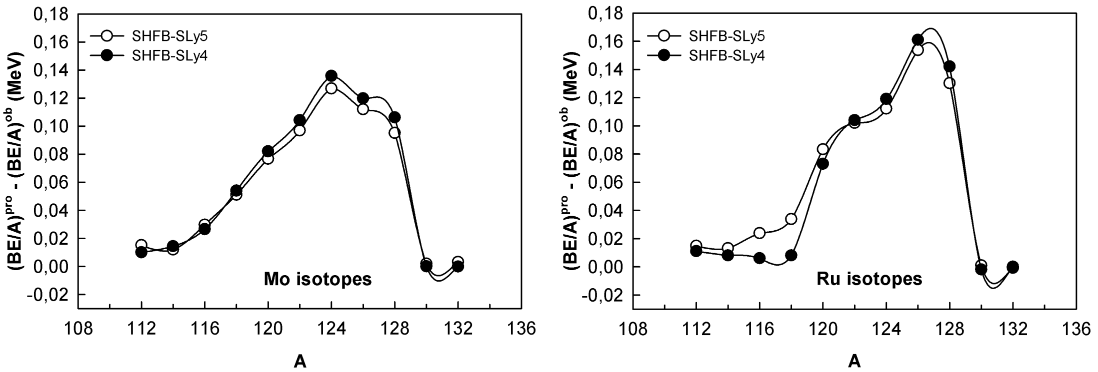

Figure 4: The prolate-oblate shape coexistance for neutron-rich Mo and Ru isotopes in HFB method

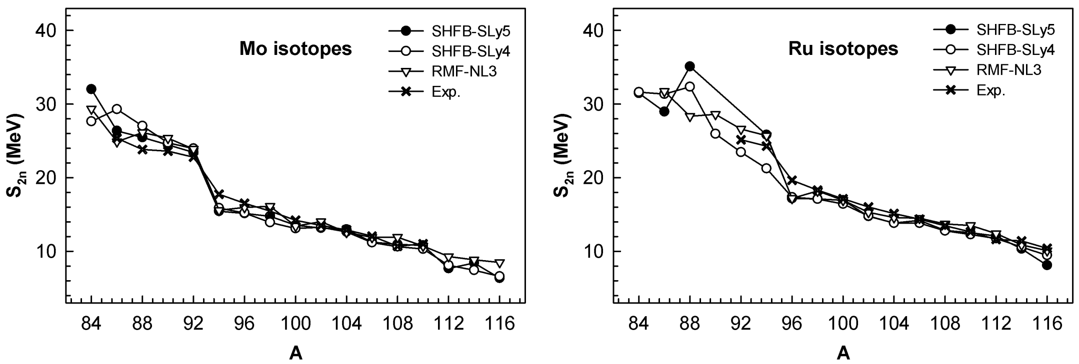

Figure 5: The calculated two-neutron separation energies for some Mo and Ru nuclei in HFB method.

The one-neutron and two-neutron separation energies are more important in investigating the nuclear shell structures. In the present work we calculated two-neutron separation energies (S_{2n}) for some Mo and Ru isotopes in both SLy4 and SLy5 parametrizations. The calculated S_{2n} for Mo and Ru isotopes as well as predictions of RMF theory and the values from available experimental results [25] are shown in Fig. 5 for comparison. The predictions of RMF theory obtained using the binding energies of Mo and Ru isotopes from Ref. [19] and $S_{2n}(Z,N) = B(Z,N) - B(Z,N-2)$ equation were calculated. As can be seen in Fig. 5, predictions of two-neutron separation energies for Mo and Ru nuclei in HFB method with Sly4 and SLy5 Skyrme forces and RMF theory with NL3 parameters set are agreement with experimental results. There are small differences between predictions of HFB method and experimental results. The approximately maximal errors of S_{2n} between the calculated results in present study and experimental results are 1.50 MeV and 0.70 MeV for Mo and Ru isotopes, respectively. In particular, the abrupt decrease of S_{2n} of Mo and Ru isotopes in both SLy4 and SLy5 parametrizations at neutron number N = 50 corresponding to shell effect which is enhanced when neutrons form closed shell that cannot be described satisfactorily in a mean field formalism [26, 27] is reproduced as larger than the observed one.

Table 2: The calculated proton (Q_p), neutron (Q_n), and total (Q_T) quadrupole moment values for some Mo and Ru nuclei in SLy4 Skyrme force.

Neutron Number	Mo Isotopes (Z=42)			Ru Isotopes (Z=44)		
	Q_p(barn)	Q_n(barn)	Q_T (barn)	Q_p(barn)	Q_n(barn)	Q_T (barn)
40	4.873	4.292	9.166	3.648	3.307	6.955
42	5.303	5.067	10.369	2.621	2.480	5.101
44	1.698	1.711	3.408	0.583	0.558	1.141
46	0.041	0.048	0.089	8.150	8.329	16.479
48	0.006	0.007	0.012	0.274	0.283	0.557
50	0.003	0.003	0.006	0.006	0.005	0.011
52	0.010	0.015	0.025	0.557	0.677	1.233
54	0.500	0.783	1.283	1.352	1.768	3.120
56	1.397	2.183	3.580	1.766	2.478	4.244
58	2.840	4.066	6.906	2.035	2.889	4.925
60	3.413	5.131	8.544	2.786	4.109	6.895
62	3.761	5.805	9.566	3.204	4.987	8.191
64	3.860	6.139	9.988	3.320	5.300	8.620
66	3.820	6.224	10.044	3.295	5.384	8.679
68	3.743	6.242	9.985	3.198	5.370	8.568
70	3.674	6.224	9.898	2.984	5.028	8.013

SUMMARY AND CONCLUSIONS

The HFB method with SLy4 and SLy5 Skyrme forces were employed to investigate the ground-state properties of axially deformed even-even Mo and Ru isotopic chains. Binding energies, deformation properties, charge radii, neutron radii and two-neutron separation energies for Mo and Ru isotopes were obtained. The results of these calculations were compared with empirical data available on the binding energies per nucleon, quadrupole deformations and two-neutron separation energies. The HFB method produced the binding energies per nucleon of Mo and Ru nuclei very well. It can be noted that the results of the BE/A and S_{2n} of the both nuclei in the SLy5 parametrization which includes tensor term are closer then the those of SLy4 parametrization to experimental ones although the results of the both parametrizations are close to each other. The neutron radii for both Mo and Ru isotopic chains showed a king at four and six neutrons below the closed neutron shell (N = 50), respectively. This situation is needed further investigation. The quadrupole deformations of Mo and Ru nuclei are well described with small differences from experimental results. Because of these reasons, it is possible concluded that the HFB method with SLy4 and SLy5 Skyrme forces is capable of describing ground-state properties of Mo and Ru nuclei.

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