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### Electrical transport properties of liquid alloys

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## Electrical transport properties of liquid alloys

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The electrical transport properties namely the electrical resistivity ( $\rho$ ), the thermoelectric power (TEP) and the thermal conductivity ( $\sigma$ ) of several polyvalent alloys like  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  were calculated from the pseudopotential form factors and Percus-Yevic (PY) hard sphere structure factors of Ashcroft and Langreth. The well-recognized empty core model (EMC) potential of Ashcroft is used for the first time with seven local field correction functions due to Hartree (H), Hubbard–Sham (HS), Vashista–Singwi (VS), Taylor (T), Ichimaru–Utsumi (IU), Farid *et al.* (F) and Sarkar *et al.* (S) in the present computation and found suitable for such study. It is concluded that the comparison of present and experimental findings is highly encouraging.

*Keywords:* Model potential; Electrical resistivity; Binary alloys

### 1. Introduction

During the last several years there has been an increasing interest in the properties of non-crystalline conductors such as liquid metals and liquid metallic alloys. Such a liquid exhibits metallic as well as fluid-like behaviour and hence can help to make a link between the theory of the liquid states and the theory of the electronic states in metals. And hence the study of electrical transport properties of liquid metals and their alloys remains one of the favourite quantities either experimentally or theoretically [1–11]. It was found that the electrical resistivities of the alloys obey two rules: (i) Nordheim's rule [12] and (ii) Linde's rule [13]. In Nordheim's rule the resistivity of liquid alloys depends directly on the product of the atomic concentrations in the percentage of the guest and host elements [12]. While according to Linde's rule [13], the resistivity derivative with respect to atomic concentration is directly proportional to the difference of the variables of the guest and host elements.

Despite the rich accumulation of experimental studies, the atomistic approach to the problem of the liquid metals had been very slow in progress until Ziman [14] proposed the theory of electrical resistivity of liquid metals. Basically, there are three approaches for the theoretical investigations of transport properties of liquid metals: one is based on the nearly free electron picture [14], second one is the finite

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mean-free path approach [5] and the third is based on tight-binding approximation [15]. The tight-binding approach usually involves either the average  $T$ -matrix approximation or the coherent potential approximation. A self-consistent approach corresponding to the finite mean free-path is taking account of finite uncertainty in the electron momentum. In this article, we report the electrical resistivity ( $\rho$ ), the thermoelectric power (TEP) and the thermal conductivity ( $\sigma$ ) of several polyvalent alloys namely  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  based on the well-recognized empty core model (EMC) potential of Ashcroft [16]. Hence, both the second and the third approaches are beyond the confines of present objectives of the article as well as pseudopotential theory. So we will only be concerned and concentrate with the first approach of nearly free electron theory of Ziman [14].

In the past, Faber–Ziman [17] extended the formula for pure liquid metals easily to the binary alloys. The two important ingredients of the formula are the partial structure factors and the form factors, respectively. When one is calculating the transport properties of binary alloys, problems arise from the partial structure factors rather than from the form factors. Experimental data on the partial structure factors are scarce or have insufficient accuracy. In the present work, the partial structure factors are computed from the well-known Percus–Yevic (PY) hard sphere model of Ashcroft and Langreth [3]. Seven different types of the local field correction functions proposed by Hubbard–Sham (HS) [18,19], Vashista–Singwi (VS) [20], Taylor (T) [21], Ichimaru–Utsumi (IU) [22], Farid *et al.* (F) [23] and Sarkar *et al.* (S) [24] are employed for the first time to investigate the influence of exchange and correlation effects with reference to the static Hartree (H) [25] screening function in the present computations.

## 2. Theoretical methodology

The Faber–Ziman [17] approach of investigating electrical resistivity of liquid metals assume the model of a gas of conduction electrons that interact with and are scattered by irregularly placed metal ions. As an external electric field drives the electron through the disordered medium, the scattering determines the electrical resistance that can be calculated using perturbation theory: the transition rate from an initial state  $|\mathbf{k}\rangle$  to the final state  $|\mathbf{k} + \mathbf{q}\rangle$  on the Fermi level with the density of state is given by

$$P(\theta) = \frac{2\pi}{\hbar} |\langle \mathbf{k} + \mathbf{q} | W | \mathbf{k} \rangle|^2 \frac{1}{2} N_{\text{FE}}(E_{\text{F}}), \quad (1)$$

where  $\theta$  is the angle between  $k$  and  $k + q$ , the factor  $(1/2)$  arises from the fact that electron spin does not change on scattering. Now the conductivity in the relaxation time approximation is given by

$$\sigma = \frac{1}{3} e^2 v_{\text{F}}^2 \tau N_{\text{FE}}(E_{\text{F}}). \quad (2)$$

Here  $e$  is the electronic charge,  $v_{\text{F}}$  is the velocity of the electrons at the Fermi level and  $\tau$  is the relaxation time. The relaxation time,  $\tau$ , is given by

$$\frac{1}{\tau} = \int (1 - \cos \theta) P(\theta) d\Omega, \quad (3)$$

where  $\theta$  is scattering angle,  $\Omega$  is solid angle and  $P(\theta)$  is probability for scattering through the angle  $\theta$ .

Now assuming the free electron distribution, an expression for the electrical resistivity of liquid metal in terms of the average of the product of the structure factor and pseudopotential matrix element can be written as [1–11,14]

$$\rho = \frac{3\pi m^2}{4e^2 \hbar^3 n k_F^6} \int_0^\infty S(q) |V(q)|^2 q^3 dq \theta(2k_F - q), \tag{4}$$

where  $n$  is the electron density related to Fermi wave number and  $\theta$  is the unit step function that cuts of the  $q$ -integration at  $2k_F$  corresponding to a perfectly sharp Fermi surface.  $S(q)$  is the structure factor and  $V(q)$  is the screened ion pseudopotential form factor.

This method is initially applied to the liquid metals only, but later on the approach restructured to investigate the resistivity of  $A_{1-X}B_X$  liquid binary alloys [1–11,14]. Hence equation (4) is written as

$$\rho = \frac{3\pi m^2}{4e^2 \hbar^3 n k_F^6} \int_0^\infty \lambda(q) q^3 dq \theta(2k_F - q), \tag{5}$$

with

$$\lambda(q) = (1 - X)S_{11}V_1^2(q) + 2\sqrt{X(1 - X)}S_{11}S_{22}V_1(q)V_2(q) + XS_{22}V_2^2(q). \tag{6}$$

Here,  $V_1(q)$  and  $V_2(q)$  denote the model potentials for elements A and B,  $S_{ij}$  are the partial structure factors,  $X$  is the concentration of the second metallic component of  $A_{1-X}B_X$  mixture. Here we have used Ashcroft–Lengreth’s [3] formulations to generate the partial structure factor of the binary metallic complexes.

The expression TEP is given by [2]

$$\text{TEP} = -\left(\frac{\pi^2 k_B^2 T_K}{3|e|E}\chi\right)_{E=E_F} \tag{7}$$

with

$$\chi = 3 - 2\xi, \tag{8}$$

where

$$\xi = \frac{\lambda(q)}{\rho}. \tag{9}$$

It is well known that if a temperature gradient is applied to a metal, the conduction electrons will carry a heat current along with them even though an electric current is prevented from flowing and that indeed they are responsible for the major part of the thermal conductivity. The expression of the thermal conductivity ( $\sigma$ ) for the binary alloy can be written as [2]

$$\sigma = \left(\frac{\pi^2 k_B^2 T_K}{3|e|^2 \rho}\right). \tag{10}$$

Here,  $e$ ,  $E$ ,  $E_F$ ,  $T_K$ ,  $k_B$  and  $\chi$  are the electronic charge, energy, Fermi energy, temperature (K), the Boltzmann's constants and the term of dimensionless thermo-electric power, respectively.

In the present work, the electrical transport properties namely the electrical resistivity ( $\rho$ ), the TEP and the thermal conductivity ( $\sigma$ ) of several polyvalent alloys have been calculated by applying Ashcroft's well-known empty core (EMC) model potential [16] including seven different types of the local field correlation functions [18–25]. The form factor explored in the present investigation is of the form [16],

$$W(q) = \frac{-4\pi Ze^2}{\Omega_0 q^2 \varepsilon(q)} \cos(qr_C), \quad (11)$$

where,  $Z$  is the valence,  $\Omega_0$  is the atomic volume,  $r_C$  is the parameter of the potential and  $\varepsilon(q)$  is the modified Hartree dielectric function [27]. The parameter of the potential  $r_C$  may be set from appropriate experimental information (e.g., the Fermi surface or ionization energy). In this instance, it was determined by the known electrical resistivities of the pure liquid metals at the melting points.

### 3. Results and discussion

The input parameters and constants used in the present computations are narrated in table 1. The computed results of electrical properties namely the electrical resistivity ( $\rho$ ), the thermoelectric power (TEP) and the thermal conductivity ( $\sigma$ ) of  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  binary alloys are displayed in figures 1–6.

The concentration dependence of the electrical resistivity ( $\rho$ ) is examined by varying  $X=0$  to  $X=1$  in the step size of 0.1. The results for the presently calculated electrical resistivities ( $\rho$ ) for  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  systems at  $300^\circ\text{C}$  is shown with the experimental data [26, 27] in figures 1–3. From the figures 1 and 2 it is seen that, among the seven employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives the minimum numerical value of the electrical resistivity, while the local field correction function due to F gives the maximum value. The present findings of the electrical resistivity ( $\rho$ ) of  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  binary alloys due to HB, VS, T, IU and S local field correction functions are lying between H and F functions. The linear nature is almost found for  $\text{In}_{1-x}\text{Bi}_x$  alloys and the results due to HB screening are found in good agreement with the experimental data [26].

The packing fraction,  $\eta$ , for the alloys was obtained by taking a linear average of the two components at each composition. Ashcroft and Lengreth [3] pointed out that the packing fraction,  $\eta$ , calculated by comparison of the working temperature and

Table 1. The input parameters and constants.

Metal	Z	Hard sphere		$\eta$	$r_C$ (au)	$\Omega_0$ (au)
		Diameter (D) (au)				
In	3	5.4424		0.42	1.3379	244.84
Sn	4	5.5180		0.44	1.3285	194.64
Bi	5	5.8959		0.456	1.5175	206.48

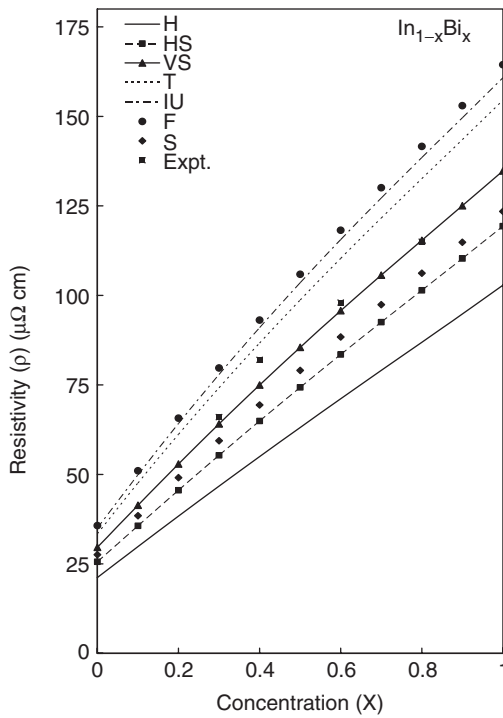


Figure 1. Electrical resistivity ( $\rho$ ) of In<sub>1-x</sub>Bi<sub>x</sub> binary mixture.

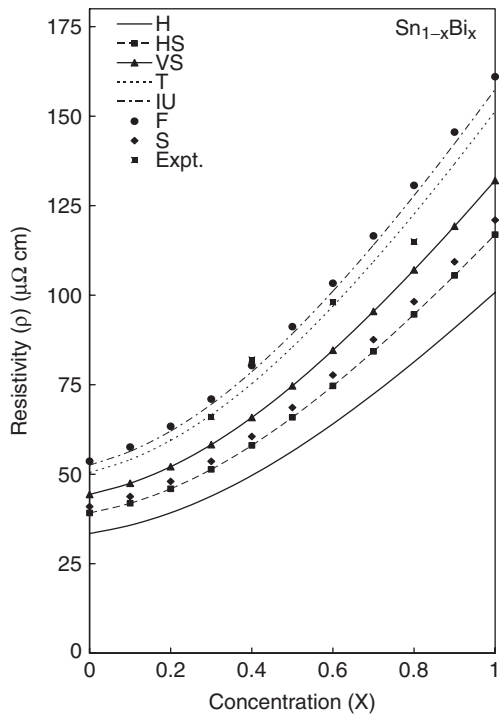


Figure 2. Electrical resistivity ( $\rho$ ) of Sn<sub>1-x</sub>Bi<sub>x</sub> binary mixture.

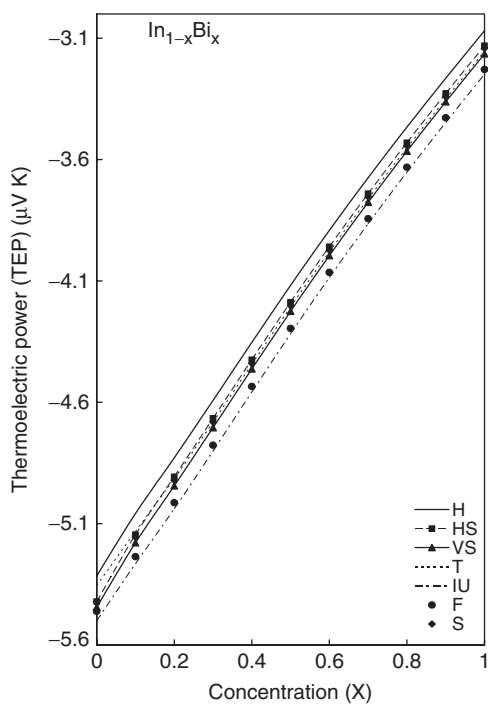


Figure 3. Thermoelectric power (TEP) of  $\text{In}_{1-x}\text{Bi}_x$  binary mixture.

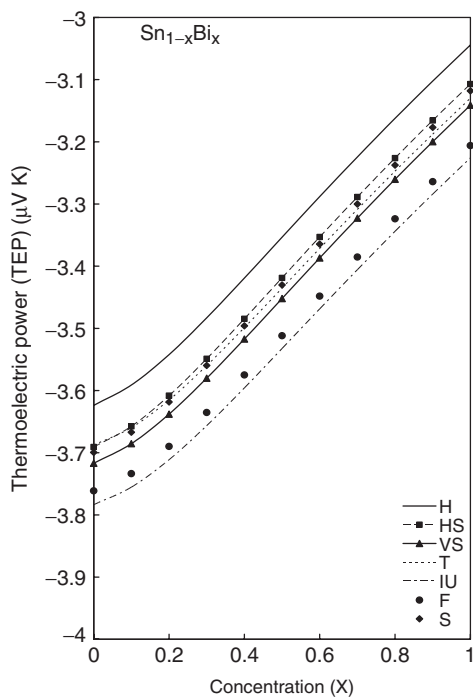


Figure 4. Thermoelectric power (TEP) of  $\text{Sn}_{1-x}\text{Bi}_x$  binary mixture.

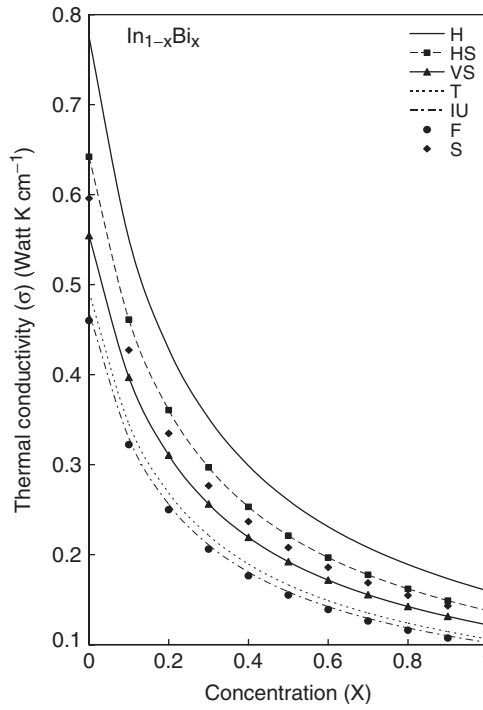


Figure 5. Thermal conductivity ( $\sigma$ ) of In<sub>1-x</sub>Bi<sub>x</sub> binary mixture.

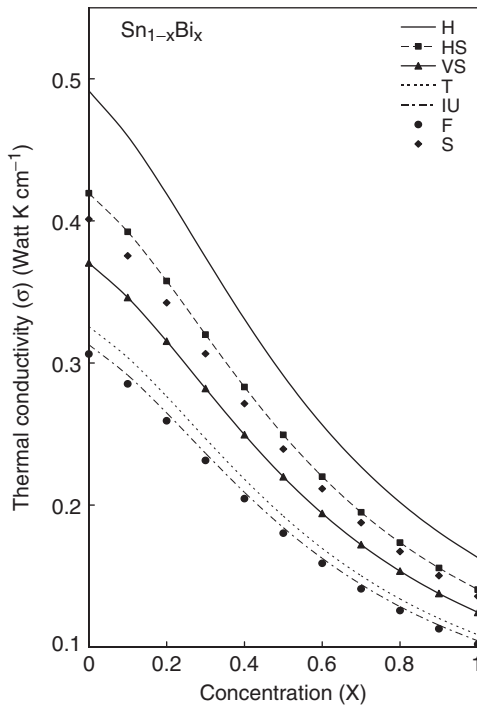


Figure 6. Thermal conductivity ( $\sigma$ ) of Sn<sub>1-x</sub>Bi<sub>x</sub> binary mixture.



the liquidus temperature using  $d\eta/dT$  for the components does not differ significantly from the linear combination of the pure component packing fraction. The present results are found in qualitative agreement with the available experimental findings [26,27]. One interesting feature is noted herewith as concentration  $X$  of the element B increases, electrical resistivity ( $\rho$ ) of the system increases.

In comparison with the presently computed results of the electrical resistivity ( $\rho$ ) from static H function, the percentile influences for  $\text{In}_{1-x}\text{Bi}_x$  alloys of HB, VS, T, IU, F and S functions are of the order of 16.02–20.76%, 31.03–39.83%, 50.20–59.58%, 56.32–67.43%, 59.86–71.34% and 20.04–28.91%, respectively. While those influences found for  $\text{Sn}_{1-x}\text{Bi}_x$  binaries are of the order of 16.02–17.319, 31.01–32.82%, 50.15–51.67%, 56.23–58.37%, 59.37–61.77% and 20.03–22.55%, respectively.

The qualitative agreement with the experimental data may be indicative of the free electron behaviour of these mixtures in the whole concentration range. Here also, the calculated electrical resistivities of the  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  systems increase like alkali–alkali systems. The peak of the curve increases with the increase of their electronegativity differences. The present study indicates the free electron behaviour of these mixtures in the whole composition range and all the constituent atoms are randomly distributed in the system.

The TEP for  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  binary systems are displayed in figures 3 and 4. It is seen that, as the concentration  $X$  of the element B increases, the TEP decreases and reaches the maximum value; after that the further increase in  $X$  increases the TEP of the system. Also, among the seven employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives the maximum numerical value of the TEP, while the local field correction function due to F gives the minimum value. The present findings of the TEP of  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  binary alloys due to HB, VS, T, IU and S local field correction functions are lying between H- and F functions. The linear nature is almost found for  $\text{In}_{1-x}\text{Bi}_x$  alloys. The experimental or theoretical data of TEP are not available for the further comparison. In the study of the TEP for binary alloys, when two different metals are placed in contact, charge flows from one to another until a potential difference is set up such that  $E_F^A = E_F^B$ .

In comparison with the presently computed results of the TEP from static H function, the percentile influences for  $\text{In}_{1-x}\text{Bi}_x$  alloys of HB, VS, T, IU, F and S functions are of the order of 1.61–2.01%, 2.39–3.11%, 0.75–2.76%, 3.49–5.85%, 2.75–5.21% and 2.01–2.37%, respectively. While those influences found for  $\text{Sn}_{1-x}\text{Bi}_x$  binaries are of the order of 1.85–2.06%, 2.57–3.18%, 1.76–2.81%, 4.41–6.97%, 3.79–5.31% and 2.09–2.42%, respectively.

The thermal conductivity ( $\sigma$ ) for  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  binary systems are shown in figures 5 and 6. It is noted that as the concentration  $X$  of the element B increases, the thermal conductivity ( $\sigma$ ) decreases. Also, among the seven employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives the maximum numerical value of the thermal conductivity ( $\sigma$ ), while the local field correction function due to F gives the minimum value. The present findings of the thermal conductivity ( $\sigma$ ) of  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  binary alloys due to HB, VS, T, IU and S local field correction functions are lying between H and F functions. The experimental or theoretical data of thermal conductivity ( $\sigma$ ) are not available for the further comparison.

In comparison with the presently computed results of the thermal conductivity ( $\sigma$ ), from static H function, the percentile influences for  $\text{In}_{1-x}\text{Bi}_x$  alloys of HB, VS, T, IU, F and S-functions are of the order of 13.78–15.83%, 23.67–27.90%, 33.44–37.33%, 36.01–40.27%, 37.45–41.64% and 16.66–21.87%, respectively. While those influences found for  $\text{Sn}_{1-x}\text{Bi}_x$  binaries are of the order of 13.80–14.67%, 23.68–24.33%, 33.37–34.08%, 35.95–36.79%, 37.42–38.20% and 16.69–18.39%, respectively.

The numerical values of the electrical transport properties namely the electrical resistivity ( $\rho$ ), the thermoelectric power (TEP) and the thermal conductivity ( $\sigma$ ) are found to be quite sensitive to the selection of the local field correction function and showing a significant variation with the change in the function. Thus, the calculations of the electrical transport properties namely the electrical resistivity ( $\rho$ ), the thermoelectric power (TEP) and the thermal conductivity ( $\sigma$ ) are one of the sensitive tests for the proper assessment of the form factor of the model potential and in the absence of experimental information such calculations may be considered as one of the guidelines for further investigations either theoretical or experimental.

It is apparent that for all cases, using the resistivity model of Ashcroft and Langreth [3], better calculated agreement with experimental values was obtained by allowing variation in atomic volume. One could conclude from this information that structure information in resistivity models seems to be required.

#### 4. Conclusions

Finally, we concluded that the electrical transport properties namely the electrical resistivity ( $\rho$ ), the thermoelectric power (TEP) and the thermal conductivity ( $\sigma$ ) of several polyvalent alloys namely  $\text{In}_{1-x}\text{Bi}_x$  and  $\text{Sn}_{1-x}\text{Bi}_x$  are reported for the first time using EMC model potential and Percus–Yevic (PY) hard sphere model with seven different types of local field correction functions. The EMC model potential with more advanced IU, F and S local field correction functions generate consistent results regarding the electrical transport properties. Hence, the EMC model potential is found suitable for studying the electrical transport properties of polyvalent alloys. Also, the present investigation predicts that the present study of the electrical transport properties is sensitive to the selection of the proper local field correction function.

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