

Theoretical attempt to predict the cross sections in the case of new superheavy elementsSahila Chopra,¹ Neetu Goel,¹ Manoj K. Sharma,² Peter Otto Hess,³ and Hemdeep⁴¹*Computational and Theoretical Chemistry Group, Department of Chemistry, Panjab University, Chandigarh 160014, India*²*School of Physics and Material Science, Thapar University, Patiala 147004, India*³*Instituto de Ciencias Nucleares, UNAM, 04510 Mexico-City, Mexico*⁴*Malwa College, Bondli-Samrala, Punjab 141114, India*

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For the first time, within the framework of the dynamical cluster-decay model (DCM) by Gupta and collaborators, we provide reasonable estimations for cross sections of nuclear systems which will give rise to new superheavy elements. The important point and the new approach presented in this contribution are the theoretical calculations done without tracking any reference to experimental data; i.e., these are independent calculations. We will provide a method for reasonable estimates for the cross sections of unobserved possible decay channels in a nuclear reaction. We will demonstrate the capability of the DCM to give a probable/sensible range of the cross section. This exercise of theoretical calculations within the DCM may benefit experiments for the discovery of new superheavy elements. Our results can provide hints to the experimentalist to choose proper incoming channels in order to perform experiments. We have applied this new strategy to calculate the cross sections of the already studied compound nuclei $Z = 116$ and 118 via hot fusion reactions, and observed that our calculated range of cross sections has given values within the reach of experimental studies. Both compound nuclei were studied earlier by one of the authors for the angle $\Phi = 0^\circ$, including quadrupole deformations, β_{2i} alone with “optimum” orientations ($\theta_{\text{opt.}}$). Here, we consider the same specifications in order to study the new approach using the DCM. The principal aim of this work is to study the capability of the DCM to determine the cross sections for new elements, where experimental data are not available.

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Introduction. Researchers are pursuing new discoveries of superheavy elements (SHEs) and much experimental progress has been made regarding their synthesis and related stability aspects. At present the heaviest element observed is $Z = 118$, known as ognesson (Og). Both theoreticians and experimentalists are working in this field to find the feasible incoming channels for the synthesis of new superheavy elements. In nuclear physics, several theoretical models exist which move in this direction to give predicted cross sections. In this work we discuss the predictions of new elements within the framework of the dynamical cluster-decay model (DCM). The focus of this work is to examine the most desirable characteristic of the DCM, i.e., its capability of calculating realistic or approximate cross sections for the discovery of new superheavy elements. This will give us an idea which incoming channel will accommodate new discoveries. We have taken two reactions forming $Z = 116$ ($A = 293$) [1] and $Z = 118$ ($A = 297$) [2] through the incoming channels $^{245}\text{Cm} + ^{48}\text{Ca}$ and $^{249}\text{Cf} + ^{48}\text{Ca}$, respectively. The experimental cross sections are $0.3^{+1.0}_{-0.27}$ pb for the $3n$ decay channel and 0.9 pb for the $2n$ decay channel in $Z = 118$ and 116 , respectively. Now, we have to check whether or not our estimations are close to these numbers. The purpose using these two reactions is to cross-check our results and consequently to verify the applicability of our model. Because these reactions are experimentally known, it will help us to test our new procedure.

In this study we have applied the coplanar degree of freedom (azimuthal angle; $\Phi = 0^\circ$) (see Fig. 1) along with the higher-multipole deformations $\beta_{\lambda i}$ ($\lambda = 2, 3, 4$; $i = 1, 2$), using the DCM. In our previously published paper, we discussed the proficiency of the neck-length parameter (or ΔR or reaction-time scale) in order to calculate the cross sections for still unobserved decay channels [3]. Again in this contribution we are talking about the same capability of ΔR , but with a new idea. More specifically, in this work we are calculating ΔR without pursuing the experimental number, in order to check, without any experimental data, whether or not this parameter is capable of giving any logical number.

We have calculated the cross sections of decay channels up to the allowed maximum limit of ΔR , i.e., ≈ 2 fm. The neck-length parameter (ΔR), or equivalently the barrier lowering parameter (an inbuilt property of the DCM) [4], is the backbone of our model. In order to study the relative contributions of various components (evaporation residues (ERs), fusion-fission (ff), and quasifission (qf or capture) to the fusion cross section (σ_{fusion}), Gupta and Collaborators [5–9] introduced the concept of relative preformation probability P_0 of various decay products, in their so-called the dynamical cluster-decay model. This statistical factor (P_0) gives the structural information of a compound nucleus (CN). Because of this factor the DCM is more reliable than other fission models.

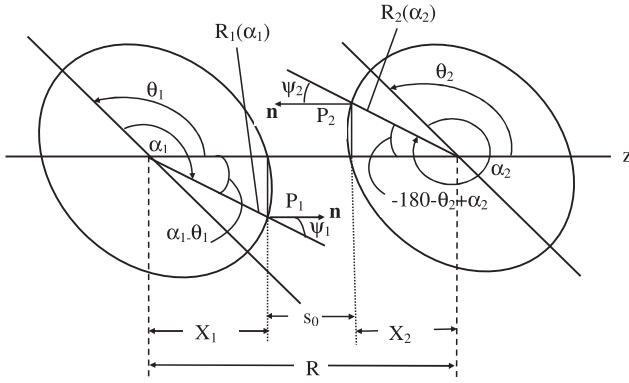


FIG. 1. Schematic configurations of two (equal/unequal) axially symmetric deformed, oriented nuclei, lying in the same plane and for various θ_1 and θ_2 values in the range 0° to 180° . The θ 's are measured counterclockwise from the colliding axis and the angles α clockwise from the symmetry axis. For details see Ref. [27].

The fusion-fission process could be said to be well established in light and medium mass dinuclear systems [10], and both BUSCO and GEMINI codes can be used for the ff process, as done in Ref. [11], though with not much success. This failure may be because the statistical fission models, for which the fission-decay of a CN is determined by the phase space (level density) available at the saddle- or scission-point configuration, are lacking in terms of not including more explicitly the structure effects of the compound nucleus (CN). Using P_0 , the proposed DCM treats all the processes of evaporation residues (ERs), IMFs, and ff within the framework of the statistical model of the decay of hot and rotating nuclei.

In the case of SHEs, we need to study an important quantity, compound nucleus survival probability (P_{surv}), which helps us to get an idea about the survival of the compound nucleus against fission, i.e., the probability of a fused system deexciting by emission of neutrons or light particles or evaporation residues (ERs) rather than fission. In the present work we are dealing with ERs and the ff region simultaneously, and both are very important for new synthesis. In a recent study, authors of the Ref. [12] discussed their dynamical investigation to understand the fission process based on the analysis of Langevin trajectories in nuclear deformation space. This study will be helpful for us if we would like to discuss our results with compact theta (θ) and noncoplanar configurations ($\Phi \neq 0$). The aim of this study is to give sensible predicted cross sections in the case of unobserved new elements. A number of theoretical works have been published studying synthesis of SHEs, but our idea is somewhat different.

In the case of $Z = 120$ [4] we have calculated the evaporation residues using the approach of Ref. [13], and we found there is a similarity between the ΔR of $Z = 118$ and $Z = 120$ (discussed in the calculations section). In our calculations, we have followed the important theoretical concepts concerning the synthesis of SHEs to determine the values of ΔR . That is, we determine whether or not evaporation residue decay is possible in the case of SHEs, and the number and type of ERs. Using the DCM, we have already studied a number of

reactions for superheavy elements and all results are in good agreement with the experimental data. Therefore, from the DCM literature on SHEs, we have found a particular range for the neck-length parameter, which always is different for light mass systems compared to heavy mass and superheavy elements. Another important point of this work is considering proper incoming channels for the synthesis of new SHEs. We have published a few papers regarding compound nucleus fusion and survival probability, P_{CN} and P_{surv} respectively [14–17]. On the basis of these quantities we can decide about the probable target and projectile combinations to consider for new discoveries.

The dynamical cluster-decay model (DCM). The dynamical cluster-decay model (DCM) of Gupta and collaborators [8,9] is based on the dynamical or quantum mechanical fragmentation theory (QMFT), in turn based on the two-center shell model (TCSM), used as an average two-body potential within the Strutinsky macroscopic-microscopic method. This theory uses the collective coordinates of mass (and charge) asymmetries η (and η_Z) [$\eta = (A_1 - A_2)/(A_1 + A_2)$, $\eta_Z = (Z_1 - Z_2)/(Z_1 + Z_2)$], and relative separation R , with multipole deformations up to hexadecupole $\beta_{\lambda i}$ ($\lambda = 2, 3, 4$; $i = 1, 2$) and orientations θ_i . In terms of these coordinates, we define the compound nucleus decay cross section for ℓ partial waves as the compound nucleus decay/formation cross section of fragments for ℓ partial waves, within the DCM for each pair of exit/decay channels:

$$\sigma_{(A_1, A_2)} = \frac{\pi}{k^2} \sum_{\ell=0}^{\ell_{\text{max}}} (2\ell + 1) P_0 P, \quad k = \sqrt{\frac{2\mu E_{c.m.}}{\hbar^2}}, \quad (1)$$

where P_0 is the fragment preformation probability, referring to the η motion at fixed R value, and P is the barrier penetrability, referring to R motion for each η value, both dependent on T and ℓ . The reduced mass $\mu = mA_1A_2/(A_1 + A_2)$ with m as the nucleon mass. ℓ_{max} is the maximum angular momentum, defined for light-particle evaporation residue cross section $\sigma_{ER} \rightarrow 0$. Then, it follows from (1) that

$$\sigma_{ER} = \sum_{A_2=1}^4 \sigma_{(A_1, A_2)} \text{ or } = \sum_{x=1}^4 \sigma_{x_n} \quad (2)$$

and

$$\sigma_{ff} = 2 \sum_{A/2}^{A/2+20} \sigma_{(A_1, A_2)}. \quad (3)$$

Thus, using Eq. (1) in Eqs. (2) and (3), the DCM predicts not only the total fusion cross section σ_{fusion} , i.e., the sum of the cross sections of constituents ER, ff, and qf, but also includes the cross sections of σ_{ER} , σ_{ff} and σ_{qf} channels. In Eq. (1), η and R motions are taken to be decoupled, though in general they are coupled, as justified in Refs. [18–21], such that the stationary Schrödinger equation for the coupled η and R coordinates (with η_Z coordinate minimized, and hence kept fixed) is given by

$$H(\eta, R)\psi(\eta, R) = E\psi(\eta, R) \quad (4)$$

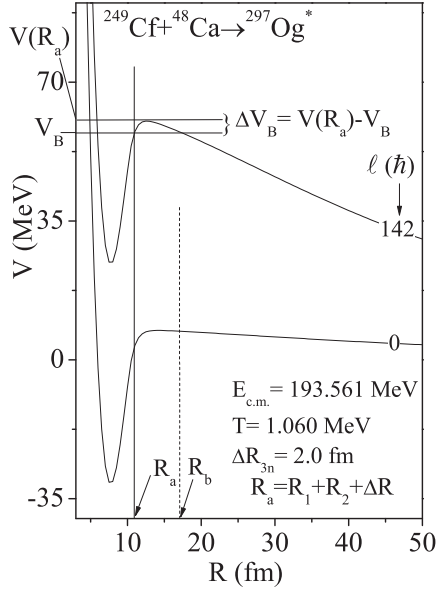


FIG. 2. Scattering potential $V(R)$ for $3n$ emission from $^{297}\text{Og}^*$ formed in $^{249}\text{Cf} + ^{48}\text{Ca}$ at $E_{c.m.} = 193.561$ MeV, plotted for $\ell_{\max} = 142\hbar$ and zero values. The definitions of the first turning point R_a , equivalently the neck-length parameter, and “barrier lowering” are also shown.

with the Hamiltonian constructed as

$$H(\eta, R) = E(\eta) + E(R) + E(\eta, R) + V(\eta) + V(R) + V(\eta, R). \quad (5)$$

Here, E refers to the kinetic energy expressed in terms of mass parameters B_{ij} ; $i, j = R, \eta$ [22–24]. $V(\eta, R, T)$, the T -dependent collective potential energy, is calculated as per the Strutinsky renormalization procedure ($B = V_{LDM} + \delta U$), using the T -dependent liquid drop model energy $V_{LDM}(T)$ of Davidson *et al.* [25]. For the kinetic energy part, the mass parameters $B_{\eta\eta}$ used are the smooth classical hydrodynamical masses [22]. Then, the Hamiltonian (5), for each ℓ value, on using the Pauli-Podolsky prescription [26], takes the form

$$H = -\frac{\hbar^2}{2\sqrt{B_{\eta\eta}}} \frac{\partial}{\partial \eta} \frac{1}{\sqrt{B_{\eta\eta}}} \frac{\partial}{\partial \eta} - \frac{\hbar^2}{2\sqrt{B_{RR}}} \frac{\partial}{\partial R} \frac{1}{\sqrt{B_{RR}}} \frac{\partial}{\partial R} + V(\eta) + V(R). \quad (6)$$

The Schrödinger equation (4) becomes separable in η and R coordinates, and its solutions are $|\psi(\eta)|^2$ and $|\psi(R)|^2$, respectively, providing the probabilities P_0 and P of Eq. (1). $P_0(A_i)$ is obtained at a fixed $R = R_a$ (see Fig. 2), the first turning point(s) of the penetration path(s) for different ℓ values. Thus, R_a introduces a T -dependent parameter $\Delta R(T)$, the neck-length parameter, which assimilates the deformation and neck formation effects between two nuclei [28–30]. Note that ΔR introduces an inbuilt property of “barrier lowering” [8,9]. Next, the penetrability P is given by the WKB integral, which is solved analytically [31,32], instead of by solving the corresponding radial Schrödinger equation in R . For detailed methodology, see Refs. [14,15].

Calculations and results. In this section, we will present and discuss our calculations using the dynamical cluster-decay model (DCM) in order to study its application for the discovery of new elements. We have taken two super-heavy compound nuclei $Z = 116$ ($A = 293$) [1] and 118 ($A = 297$) [2], via the incoming channels $^{245}\text{Cm} + ^{48}\text{Ca}$ and $^{249}\text{Cf} + ^{48}\text{Ca}$, respectively. In this work, our DCM calculations have shown potential for the prediction of approximate and sensible cross sections for new discoveries. We have studied these reactions within the framework of the DCM along with the following set of parameters: coplanar degree of freedom $\Phi = 0^\circ$, higher-multipole deformations $\beta_{\lambda i}$ ($\lambda = 2, 3, 4$; $i = 1, 2$), and “optimum” orientations (θ_{opt}). In our previous work for the case of $Z = 122$ [33], we calculated the cross sections for unobserved evaporation residues (ERs) at all energies. There, we had only one experimental data point and at other center-of-mass energies ($E_{c.m.}$) we calculated the DCM-predicted or estimated cross sections. In the case of $^{196}\text{Pt}^*$, we have did similar exercise for one $E_{c.m.}$, where we had data at four other energies, and our DCM-calculated number followed the same trend other results. Now, In this work we have taken a different approach: instead of calculating ΔR by adjusting to the experimental data (as done in previous contributions), we have extracted the cross sections according to the values of ΔR (emerging from the concepts of the DCM). Then the results of our calculations are in good agreement with the experimental data. We performed our calculations according to the theoretical aspects in the case of SHEs and using the ideas about the decay processes within the framework of the DCM. In the calculated results for SHEs via the DCM, we have noticed a particular tendency of neck-length parameter (ΔR) to move in a fixed range, i.e., ≈ 1.2 to 2.0 fm. The maximum value of ΔR depends upon the penetration probability P , which can not be unity, and also on the scattering potential graph, where the area under the curve should be between the two turning points (R_a and R_b). Note in Fig. 2 that the neck-length parameter ΔR also contains the effects of “barrier lowering” for each decay channel, defined for each ℓ as the difference between $V_B(\ell)$ and $V(R_a, \ell)$, the actually calculated and the actually used barriers, as $V_B(\ell) = V(R_a, \ell) - V_B(\ell)$ [8,9].

Here we elaborate on why have we have considered SHEs that were already discovered. With this exercise we have confirmed our claim that the DCM-predicted cross sections follow the same trend as experiments (this work provides the cross-check of the DCM calculations. It means our method and theoretical aspects behind these calculations are in the right direction.

Figure 3 shows the DCM-predicted cross sections for $Z = 116$ and $Z = 118$ compound nuclei. For both $Z = 116$ and 118 , curves are moving towards the higher values of ΔR , i.e., from 1.2 to 2.0 fm, where 2.0 fm was taken as the maximum value or limit for ΔR according to the proximity potential. In the previously published works on the DCM, especially in the cases of SHEs, we have found that a specific range of ΔR works perfectly to reach the experimental data with adequate agreement. In this figure, we have also given two other numbers (red in color) of experimental data, which exactly fall within the range of our DCM calculations (these numbers

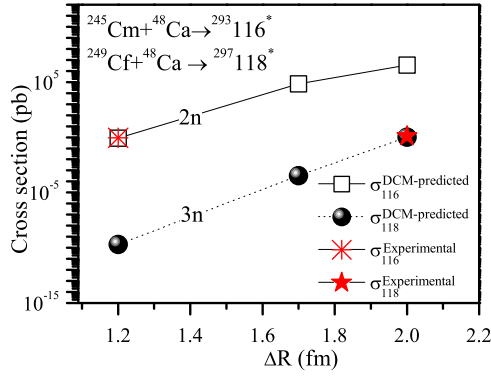


FIG. 3. DCM-predicted cross sections at different values of ΔR for $Z = 116$ [1] and $Z = 118$ [2]. Red colored values are the experimental numbers, which fall on the same curve as, or within the range of, our DCM-calculated values.

have no fixed ΔR). Here, we have kept the experimental number only for a comparison, which gives an idea about the trend of experimental data. In the DCM calculations we have shown the cross section value at three $\Delta R = 1.2, 1.7,$ and 2.0 fm. Here we mention a point about the ΔR 's: if we check the published results for $Z = 118$ [34], then ΔR must be within our mentioned range.

One important point regarding ΔR that it is a very sensitive parameter, and in our calculations we have found different values of this parameter in the simultaneous fitting of different decay channels, which we have fixed after a number of attempts, i.e., for σ_{ER} and σ_{ff} (see Table I). Table I shows how sensitive ΔR is, and that it can vary up to four decimal places if needed. A particular value of ΔR of a decay channel can change the cross section value of other decay channels in the simultaneous fittings. This outcome clearly shows that

during the fission process every decay fragment affects each other. Table I list three sets of different ΔR 's but at the same $E_{c.m.}$ (or temperature). We are using a range of ΔR to check the sensibility of our model in order to predict unobserved elements without any experimental reference. In the table it is clearly presented that the neck-length parameter shows different behavior for different compound nuclei ($Z = 116$ and 118). The point is to determine which decay fragment has to be calculated. Then we can check that for the case of $Z = 116$ formed via the $^{245}\text{Cm} + ^{48}\text{Ca}$ incoming channel, i.e., after the decay of either fragment, we obtain a stable isotope. Therefore, in this reaction we have checked that after the emission of $2n$ from $^{293}116^*$ we get $^{291}116^*$, which is more stable among all the isotopes for $Z = 116$. So, we decided to calculate the $2n$ -decay channel, using the DCM. Similarly, in the case of $Z = 118$, we have chosen the $3n$ -decay channel after the decay from $^{297}118^*$. In the case of $Z = 116$ for the fission region we used in the calculations the same $\Delta R = 0.9$ fm, but in the case of $Z = 118$ we have found two ΔR 's, for symmetric and asymmetric fission regions. These values of ΔR may vary, but not drastically if we follow the experimental data. Note that, in the case of $Z = 122$ formed via $^{58}\text{Fe} + ^{248}\text{Cm}$ [33], we have observed the σ_{ff} and σ_{qf} at five energies, where we have tentative data only at one, $E_{c.m.} = 33$ MeV. We have used the same values of ΔR at four other energies in order to predict the cross sections, i.e., $\Delta R_{ER} = 1.242$ fm and $\Delta R_{ff} = -0.1421$ fm. Similarly in the case of $Z = 120$ [4] formed via the $^{54}\text{Cr} + ^{248}\text{Cm}$ reaction, we have calculated σ_{ER} and predicted σ_{ff} . Table II shows the ΔR variations using the same approach as in this work for $Z = 118$. This observation also supports our present calculations using the DCM for predictions. Table III, gives the numbers for compound nucleus survival probability P_{surv} [15]. This statistical quantity defines the probability of excited compound nucleus reaching the ground state by neutron emission. It will

TABLE I. DCM-predicted cross sections with the included β_2 - β_4 deformations for the configuration $\Phi_c = 0^\circ$. The cross sections in boldface shows the logical number within the experimental range (may include error bar limits). ΔR is the largest for calculated ERs and smallest for ff, which suggests that the neutron emissions occurs earliest. We have shown 3-sets of the calculations with different values of ΔR within the range of $1.2 - 2.0$ fm, especially in the case of $2n$ for $Z = 116$ and $3n$ for $Z = 118$, with the other valid ΔR values allowed under the penetration probability (explained in the text).

Decay channel	ΔR (fm)	$\sigma^{\text{Calc.}}$ (pb)	ΔR (fm)	$\sigma^{\text{Calc.}}$ (pb)	ΔR (fm)	$\sigma^{\text{Calc.}}$ (pb)
$^{245}\text{Cm} + ^{48}\text{Ca} \rightarrow ^{293}116^*$						
$1n$	0.01	5.012×10^{-13}	0.01	4.999×10^{-13}	0.01	4.999×10^{-13}
$2n$	1.2	0.8	1.7	6.99×10^4	2.0	3.35×10^6
$3n$	0.9	8.917×10^{-10}	0.9	4.241×10^{-10}	0.9	4.24×10^{-10}
$4n$	0.9	5.65×10^{-14}	0.9	2.701×10^{-14}	0.9	2.701×10^{-14}
83-87	0.9	2.05 mb	0.9	2.05 mb	0.9	2.05 mb
127-141	0.9	11.7 mb	0.9	11.7 mb	0.9	11.7 mb
$^{249}\text{Cf} + ^{48}\text{Ca} \rightarrow ^{297}118^*$						
$1n$	-0.05	2.127×10^{-22}	-0.05	2.109×10^{-22}	-0.05	1.810×10^{-22}
$2n$	-0.05	2.54×10^{-28}	-0.05	2.539×10^{-28}	-0.05	2.114×10^{-28}
$3n$	1.2	2.00×10^{-10}	1.7	3.34×10^{-4}	2.0	1.06
$4n$	1.2	2.065×10^{-16}	1.7	1.11×10^{-8}	2.0	4.71×10^{-5}
84-94	-0.35	2.29×10^{-10} mb	-0.35	2.44×10^{-10} mb	-0.22	4.03×10^{-9} mb
121-143	-0.2	7.80×10^{-9} mb	-0.2	7.76×10^{-9} mb	-0.2	7.43×10^{-9} mb

TABLE II. DCM-calculated estimated/predicted cross sections for $Z = 120$ formed via the $^{54}\text{Cr} + ^{248}\text{Cm}$ reaction for best fitted ΔR (see Ref [4]).

Decay channel	ΔR (fm)	Cross section (pb)
$1n$	0.2	1.833×10^{-12}
$2n$	0.2	8.415×10^{-18}
$3n$	1.3854	0.58
$4n$	1.009	1.343×10^{-10}
predicted ff	0.5	3.54 (mb)

help us to choose proper target-projectile (t-p) combinations for new synthesis.

Summary and conclusions. In summary, we have presented a novel approach to predict the cross sections for undiscovered SHEs using the dynamical cluster-decay model. In this work, we have taken every scientific aspect to perform our calculations. This theoretical work has estimated the cross sections for unobserved possible decay channels in a nuclear reaction using a range of ΔR for the already studied compound nuclei $Z = 116$ and 118 via hot fusion reactions and our calculated range of cross sections matches the experimental studies. Also with the help of the compound nucleus survival probability we can suggest a suitable target-projectile combination to the experimentalists for new synthesis. We have done calculations only at one energy for both compound nuclei, using the proximity nuclear interaction potential of Blocki *et al.* for a coplanar ($\Phi_c = 0^\circ$) nuclear configuration. Our calculations are performed including deformation up to hexadecapole with “optimum” orientations

TABLE III. DCM-calculated compound nucleus survival probability P_{surv} for $Z = 116$ and $Z = 118$ (for more information regarding P_{surv} see Table I in Ref. [15]).

ΔR (fm)	Compound nucleus survival probability P_{surv}	
	$^{297}118$	$^{293}116$
1.2	0.249×10^{-11}	5.963×10^{-11}
1.7	0.418×10^{-05}	5.065×10^{-06}
2.0	0.848×10^{-01}	2.428×10^{-04}

of the hot fusion process. The “barrier lowering” effect is directly related to the variations of the ΔR parameter and these factors give complete information regarding the compound nucleus structure. In this contribution we have tried to develop a method to predict the cross sections for new element discoveries.

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