

**CALCULATIONS ON ELECTRON CAPTURE IN LOW  
ENERGY ION-MOLECULE COLLISIONS**

P. C. STANCIL

*Physics Division, Oak Ridge National Laboratory,  
P. O. Box 2008, Oak Ridge, TN 37831-6372, USA*

B. ZYGELMAN

*W. M. Keck Laboratory for Computational Physics, Department of Physics,  
University of Nevada, Las Vegas, NV 89154-4002, USA*

K. KIRBY

*Harvard-Smithsonian Center for Astrophysics,  
60 Garden St., Cambridge, MA 02138, USA*

Recent progress on the application of a quantal, molecular-orbital, close-coupling approach to the calculation of electron capture in collisions of multiply charged ions with molecules is discussed. Preliminary results for single electron capture by  $N^{2+}$  with  $H_2$  are presented.

## 1 Introduction

Electron capture by multiply charged ions colliding with  $H_2$  is an important process in laboratory and astrophysical plasmas. It provides a recombination mechanism for multiply charged ions in x-ray ionized astronomical environments which may have sparse electron and atomic hydrogen abundances<sup>1</sup>. In the divertor region of a tokamak fusion device, charge exchange of impurity ions with  $H_2$  plays a role in the ionization balance and the production of radiative energy loss leading to cooling<sup>2</sup>. X-ray and ultraviolet auroral emission from Jupiter is believed to be due to charge exchange of O and S ions with  $H_2$  in the Jovian atmosphere<sup>3</sup>. Solar wind ions interacting with cometary molecules may have produced the x-rays observed from Comet Hyakutake<sup>4</sup>. In order to model and understand the behavior of these environments, it is necessary to obtain total, electronic state-selective (ESS), and vibrational (or rotational) state-selective (VSS) capture cross sections for collision energies as low as 10 meV/amu to as high as 100 keV/amu in some instances.

Fortunately, charge transfer with molecular targets has received considerable experimental attention. Numerous measurements have been made with flow tubes<sup>5,6</sup>, ion traps<sup>7,8</sup>, and ion beams<sup>9,10,11</sup>. Flow tube and ion trap studies generally provide information on rate coefficients for temperatures between 300 K and 20,000 K, but the interpretation of the results is complicated by the

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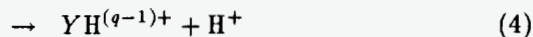
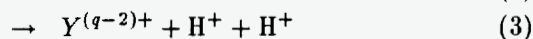
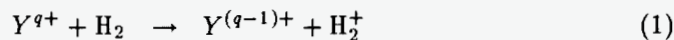
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inability to distinguish between the various product channels



referred to as single electron capture (SEC), dissociative electron capture (DiEC), double electron capture (DEC), and hydrogen abstraction (HA), respectively. HA is not considered to be an important process for multiply charged ions with  $q > 2$  and only limited knowledge<sup>6</sup> exists concerning doubly charged systems. Beam techniques can be used to obtain SEC, DEC, and in some cases DiEC cross sections, but are limited to collision energies  $E > 50$  eV/amu. Some beam techniques which use translational energy spectroscopy (TES) have been used to make ESS<sup>12,13,14</sup> and VSS<sup>15,16</sup> measurements.

While the theory and practical computation of electron capture in low-energy multiply charged ion-atom collisions has progressed to an advanced state, being routinely able to reproduce the available experimental data on total, ESS, and differential cross sections, studies of ion-molecule collisions are considerably more rudimentary. The earliest investigations of collisions of multiply charged ions with H<sub>2</sub> incorporated absorbing sphere<sup>17</sup>, electron tunneling<sup>18</sup>, and Bohr-Lindhard<sup>19</sup> models. More sophisticated close-coupling (CC) approaches, including quantum molecular-orbital CC<sup>20</sup> (MOCC), semiclassical MOCC<sup>21,22,10</sup>, and semiclassical atomic orbital CC<sup>23,24</sup> (AOCC), have only been attempted within the past decade. However, the MOCC investigations did not attempt to utilize the full triatomic potential surfaces, but instead obtained "pseudo-diatomic" potential curves by treating the target H<sub>2</sub> as an atom thereby neglecting rotational, vibrational, and collisional-orientation degrees-of-freedom. The procedure is thought to be reliable for distant collisions as the CC calculations give fair agreement with total electron capture beam measurements for  $E > 10$  eV/amu. Some collision-orientation dependence was explored in the AOCC studies, but the previous investigations have generally ignored the molecular characteristics of the target.

Singly charged systems, on the other hand, have been the subject of much theoretical activity. MOCC theories utilizing triatomic molecular surfaces have been developed to compute VSS cross sections usually within the so-called sudden approximation<sup>25,26,27</sup>. These calculations which usually consider two electronic states, each with a number of vibrational levels, have been quite successful in reproducing experimental results. It is our goal to exploit these same techniques for the study of multiply charged systems.

In this article, we report on the progress of our group in implementing a quantum-mechanical MOCC approach to the study of electron capture by multiply charged ions in collisions with molecules. We illustrate this with a preliminary investigation of SEC by  $N^{2+}$  with  $H_2$ .

## 2 *Ab Initio* Calculations of Triatomic Potential Surfaces

A key element in describing the dynamics of low-energy ion-molecule charge transfer is obtaining all the relevant adiabatic potential surfaces and wave functions for the incoming channels,  $Y^{q+} + H_2$ , as well as all the product channels listed in Eqs. 1 to 3. It is well-known from ion-atom studies that cross sections are critically sensitive to potential energy differences near avoided crossings. In order for the avoided crossings to occur at the correct nuclear geometries, asymptotic energy splittings at the separated ion-molecule limits must be described accurately. For these reasons it is important to calculate adiabatic potential surfaces for the electron capture states of the triatomic dihydrides at the highest level of accuracy possible.

We have carried out calculations of the relevant potential energy surfaces and wave functions at the configuration-interaction (CI) level, including single- and double-excitations from a multi-reference zeroth order wave function. Because of the need to describe two or more potential surfaces with the same degree of accuracy, the molecular orbitals used in constructing the CI wave functions were obtained via state-averaged multiconfiguration self-consistent field (SA/MCSCF) calculations<sup>28</sup> using the ALCHEMY II suite of programs<sup>29</sup>. Figure 1 presents the adiabatic potential curves of the lowest lying  ${}^2\Pi$  and  ${}^2\Sigma^+$  states of  $NH_2^{2+}$  in the  $C_{\infty v}$  point group, i.e., the collinear, asymmetric arrangement with the angle between the H-H axis and the N- $H_2$  axis  $\theta = 0^\circ$ . The curves were computed with  $H_2$  held at its equilibrium distance  $r_e$  and with a basis set consisting of (5s/5p/3d/1f) Slater-type orbitals (STOs) for N and (3s/2p) STOs for H. While, we have performed some calculations using a Gaussian basis in the  $C_{2v}$  point group for  $\theta = 90^\circ$ , a study of the  $BeH_2^{4+}$  system by Errea *et al.*<sup>30</sup> demonstrated that the potential surfaces and nonadiabatic couplings have a weak dependence on  $\theta$ . As such we restrict our computations to  $\theta = 0^\circ$ . Figure 1 suggests that the dominant contributions to low energy SEC will be made through the long-range  $3\ {}^2\Pi - 4\ {}^2\Pi$  avoided crossing and possibly from the short-range interaction between the  $2\ {}^2\Sigma^+$  and  $3\ {}^2\Sigma^+$  states.

Errea *et al.*<sup>30</sup>, however, found that the potential surfaces and nonadiabatic couplings have a pronounced dependence on the H-H stretching distance  $r$ . We have repeated the calculations of Figure 1 for  $1 < r < 2\ a_0$ . Figure 2 presents some results for the  $3\ {}^2\Pi$  and  $4\ {}^2\Pi$  states and demonstrates that as  $r$  increases,

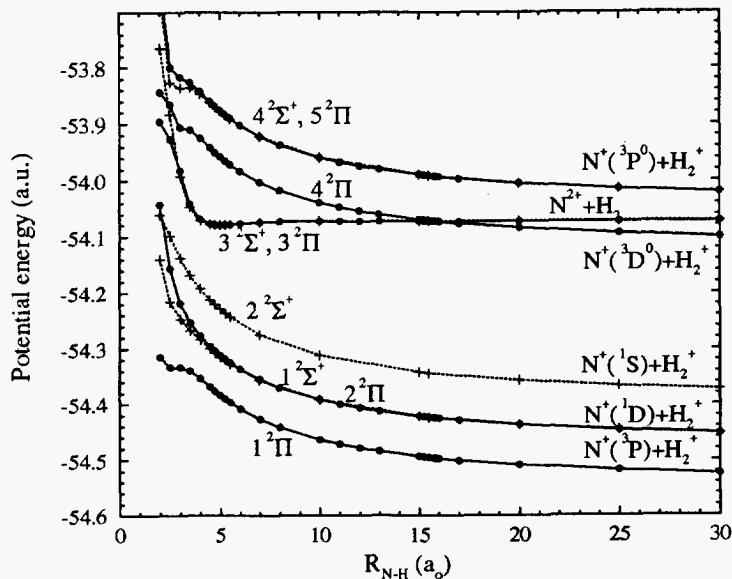


Figure 1:  $\text{NH}_2^+$  adiabatic potentials in  $C_{\infty v}$  collinear geometry ( $\theta = 0^\circ$ ) and  $r = 1.4a_0$ . Dotted lines:  $^2\Sigma^+$  states. Solid lines:  $^2\Pi$  states.

the avoided crossing distance decreases.

We did not explicitly calculate the nonadiabatic couplings, but obtained the diabatic potential, including the off-diagonal elements, by performing a unitary transformation of the adiabatic potential in a representation which diagonalizes the dipole moment matrix<sup>31,32,33</sup>. The dipole moments and transition dipole moments are obtained from the CI wave functions generated during the calculation of the potential surfaces. As with the nonadiabatic couplings<sup>30</sup>, the moments display a strong dependence on  $r$ .

### 3 Theory

The cross sections for ion-molecule SEC are calculated in a quantum-mechanical MOCC formalism which follows closely that for ion-atom electron capture described by Zygelman *et al.*<sup>34</sup>, but augmented for molecular targets following

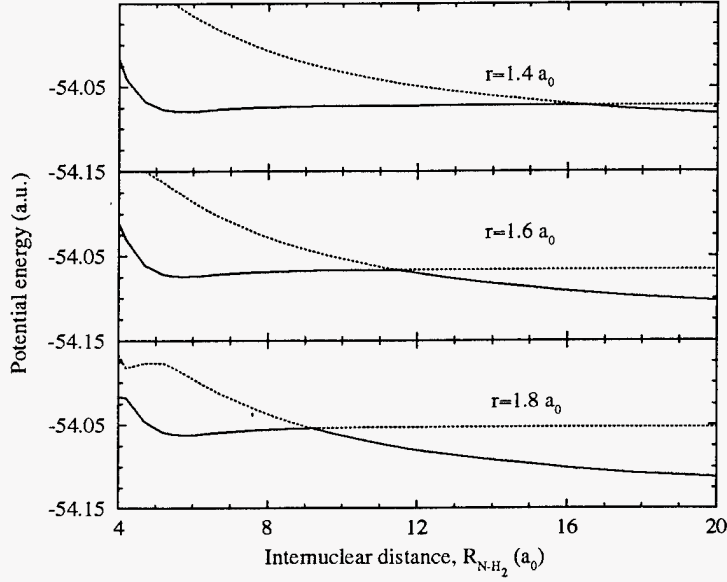


Figure 2: Dependence of the  $\text{NH}_2^+$  adiabatic potentials on the H-H stretch distance  $r$  in  $C_{\infty v}$  collinear geometry ( $\theta = 0^\circ$ ). Solid lines:  $3 \ ^2\Pi$ . Dotted lines:  $4 \ ^2\Pi$ .

Sidis<sup>25</sup>. The collision system can be represented by the Hamiltonian

$$H(\mathbf{R}, \mathbf{r}, \rho_i) = -\frac{1}{2\mu_R} \nabla_{\mathbf{R}}^2 - \frac{1}{2\mu_r} \nabla_{\mathbf{r}}^2 + H_{\text{ad}}(\rho_i | \mathbf{R}, \mathbf{r}) \quad (5)$$

with  $\mathbf{R}$  the vector between the incident ion and the  $\text{H}_2$  center of mass,  $\mathbf{r}$  the internuclear vector of  $\text{H}_2$ ,  $\rho_i$  the electronic coordinates,  $\mu_R$  the collision system reduced mass,  $\mu_r$  the  $\text{H}_2$  reduced mass, and  $H_{\text{ad}}$  the adiabatic electronic Hamiltonian of the triatomic molecule:

$$H_{\text{ad}}(\rho_i | \mathbf{R}, \mathbf{r}) \phi_\gamma(\rho_i | \mathbf{R}, \mathbf{r}) = \varepsilon_\gamma(R, r, \theta) \phi_\gamma(\rho_i | \mathbf{R}, \mathbf{r}). \quad (6)$$

$\varepsilon_\gamma(R, r, \theta)$  and  $\phi_\gamma(\rho_i | \mathbf{R}, \mathbf{r})$  are the triatomic adiabatic electronic energy and wave function, respectively, and  $\theta$  is the angle between  $\mathbf{R}$  and  $\mathbf{r}$ .

Using a perturbed-stationary state (PSS) ansatz, the total wave function

for the ion-molecule system is

$$\Psi(\mathbf{R}, \mathbf{r}, \rho_i) = \sum_{\gamma} N_{\gamma}(\mathbf{R}, \mathbf{r}) \phi_{\gamma}(\rho_i | R, r, \theta). \quad (7)$$

The lowest level of approximation is obtained by fixing  $r$  at the equilibrium nuclear separation  $r_e$  ( $1.4a_0$  for  $H_2$ ) with  $\theta = 0^\circ$  and computing the cross section following standard ion-atom MOCC methods. This is equivalent to the approaches of Gargaud and McCarroll<sup>20</sup> and Kimura *et al.*<sup>21,22,10</sup> and results in a purely electronic transition cross section  $\sigma^{\text{EL}}$ . It has been shown to give reasonable total cross sections for energies greater than  $\sim 100$  eV/amu. The highest level of approximation that we will consider involves expanding  $N$  over a complete basis of vibrational states  $v$

$$N_{\gamma}(\mathbf{R}, \mathbf{r}) = \sum_v F_{\gamma v}(\mathbf{R}) \chi_{\gamma v}(\mathbf{r}) \quad (8)$$

neglecting the rotational modes of  $H_2$ . Following Sidis<sup>25</sup>, we arrive at a PSS (diabatic representation) equation

$$\begin{aligned} & \{ \nabla_R^2 + 2\mu_R[E - \epsilon_{\gamma v}^d(R, \theta)] \} F_{\gamma v}(\mathbf{R}) \\ & = 2\mu \sum_{\gamma' \neq \gamma} \sum_{v' \neq v} \langle \chi_{\gamma v} | V_{\gamma, \gamma'}^d(R, r, \theta) | \chi_{\gamma' v'} \rangle F_{\gamma' v'}(\mathbf{R}) \end{aligned} \quad (9)$$

where the brackets refer to integration over  $r$ . Eq. 9 assumes the infinite order sudden approximation (IOSA) which is appropriate when the rotational periods are much longer than the collision time<sup>25</sup>. Following a partial-wave decomposition of  $\mathbf{F}$ , Eq. 9 can be used to obtain VSS cross sections  $\sigma_{v, v'}^{\text{IOSA}}$  which are probably reliable for energies much greater than 0.01 eV/amu.

If the collision time scale is much shorter than the vibrational period, a Franck-Condon-type approximation can be made:

$$\langle \chi_{\gamma v} | V_{\gamma, \gamma'}^d(R, r, \theta) | \chi_{\gamma' v'} \rangle \rightarrow V_{\gamma, \gamma'}^d(R, r, \theta) \langle \chi_{\gamma v} | \chi_{\gamma' v'} \rangle. \quad (10)$$

where  $\langle \chi_{\gamma v} | \chi_{\gamma' v'} \rangle$  is the square-root of the Franck-Condon (FC) factor for the overlap of the  $H_2$  and  $H_2^+$  vibrational wave functions. The approximation also gives a VSS cross section  $\sigma_{v, v'}^{\text{VSA}}$ . It may be applicable for  $E > 50$  eV/amu and we refer to it as a vibrational sudden approximation (VSA). An alternative approximation, the centroid approximation (CA), can give a VSS cross section by merely multiplying the electronic cross section by a FC factor

$$\sigma_{v, v'}^{\text{CA}} = \sigma^{\text{EL}} \langle \chi_{\gamma v} | \chi_{\gamma' v'} \rangle^2. \quad (11)$$

We note that the CA and VSA are not equivalent. The FC factors for  $H_2$  ionization would imply that the dominant VSS cross section would be for capture into  $H_2^+(v' = 2)$  followed by  $v' = 1, 3, 4, 0, \dots$ , independent of collision energy. A similar formalism for the various approximations has been outlined by Errea *et al.*<sup>35</sup>, but within a semiclassical impact-parameter picture.

#### 4 Results and Discussion

We present in Figure 3 SEC cross sections for collisions of  $N^{2+}$  with  $H_2$  calculated in the electronic approximation, VSA, and IOSA. The results are compared to the ion beam measurements of Wilkie *et al.*<sup>36</sup> for total SEC obtained between 43 and  $14 \times 10^3$  eV/amu. For lower collision energies, a cross section can be estimated from the experimental rate coefficient of Fang and Kwong<sup>37</sup> at  $\sim 2900$  K. No measurements of VSS cross sections are available, but Burns *et al.*<sup>38</sup> have made some relative ESS measurements between 125 and 570 eV/amu.

For capture into  $N^+(^3D)$  via the  $^2\Pi$  channels,  $\sigma^{EL}$  with  $r = r_e$  is in fair agreement with the measurements of Wilkie *et al.*<sup>36</sup>, but decreases rapidly with decreasing energy to give a negligible cross section at thermal energies. This is a consequence of the avoided crossing occurring at  $R \sim 16a_0$  as shown in Figure 2. However, the asymptotic energies for  $r = r_e$  may not adequately describe the energetics of the collision. Shifting the potential curves to give asymptotic energies corresponding to the  $H_2(v = 0)$  and  $H_2^+(v' = 0)$  vibrational energies increases the low energy cross sections considerably while having little effect at high energies. Capture into  $N^+(^1S)$  is typically an order of magnitude smaller than into  $N^+(^3D)$  for collision energies above 10 eV/amu with  $r = r_e$ , while shifting its potential curves to the asymptotic vibrational energies increases the high energy portion of the cross section.

Since Figure 2 demonstrates that the  $3^2\Pi - 4^2\Pi$  avoided crossing distance migrates to smaller, more optimal values, with increasing  $r$ ,  $\sigma^{EL}$  for  $r = 1.6$  and  $1.8a_0$  are displayed in Figure 3. While the cross section above 50 eV/amu has only a minor  $r$  dependence, the low energy cross section increases with  $r$ , particularly below 1 eV/amu. A similar  $r$  dependence was noted for the  $Be^{4+} + H_2$  system by Errea *et al.*<sup>35</sup> in the electronic approximation. Additional calculations in the electronic approximation for  $r = 1.6$  and  $1.8a_0$  were also performed, but with the potential curves shifted to the asymptotic vibrational energies as discussed above for  $r = 1.4a_0$ . At low energies the cross section is seen to increase with  $r$  reflecting the increase of the coupling with  $r$ . The very different behavior of the cross sections at low and high energy is a consequence of two different interaction regions: long- and short-range, respectively. While



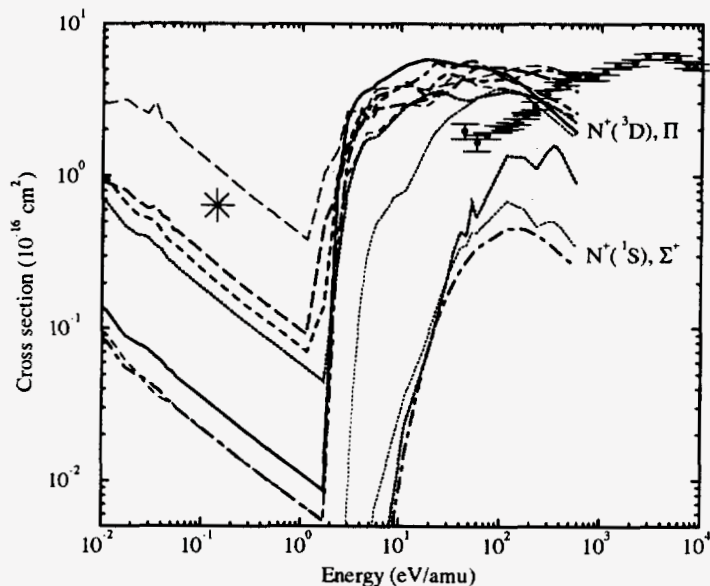


Figure 3: Single electron capture cross sections for collisions of  $N^{2+}$  with  $H_2$ . Experiment: Wilkie *et al.*<sup>36</sup> (filled circles), Fang and Kwong<sup>37</sup> (star). Theory in the electronic approximation (thin lines; thick lines with asymptotic vibrational energies) with  $\theta = 0^\circ$  and  $r = 1.4a_0$  (dotted line),  $r = 1.6a_0$  (short dash line),  $r = 1.8a_0$  (long dash line); VSA (thick dot-dash line); IOSA (thick full line).

the electronic approximation may not be valid below  $\sim 100$  eV/amu, the low energy results are presented to illustrate the dependence on asymptotic energies and  $r$ .

We have performed calculations of VSS cross sections for capture into  $v' = 0-4$  in the VSA with  $r = 1.4a_0$ . Only total cross sections are presented in Figure 3. For collision energies below  $\sim 5$  eV/amu, the dominant vibrational channels in decreasing order are  $v' = 0, 1, 2, 3, 4$  for capture into  $N^+(^3D)$ . This is in disagreement with CA expectations which predicts the order  $v' = 2, 1, 3, 4, 0$ , solely determined from the relative FC factors. This disagreement between CA and VSA suggests the vibrational distribution depends not only on FC factors, but also on the asymptotic energy defects. As  $v'$  increases, the avoided crossing distance, for capture into the  $4\ ^2\Pi$  channel, increases. For larger energies, the cross sections for capture into the individual vibrational levels

become comparable. Similar discrepancies with a CA vibrational distribution have been observed in VSS measurements<sup>15,16,13</sup>. The VSA predicts that total capture into  $N^+(^3D)$  is generally an order of magnitude larger than into  $N^+(^1S)$  over the considered energy range.

VSS calculations in the IOSA have been performed by solving Eq. 9 for the  $^2\Pi$  channels including  $v' = 0-4$ . The total and VSS cross sections are slightly larger than obtained by the VSA, but the vibrational distributions are comparable. The total IOSA SEC cross section, shown in Figure 3, is an order of magnitude smaller than the inferred Fang and Kwong<sup>37</sup> measurement. However, their measurement can not resolve the products given in Eqs. 1 through 4 and may be dominated by DEC and/or DiEC. All of the calculated cross sections are typically a factor of 1.5-3 times larger than the SEC measurements of Wilkie *et al.*<sup>36</sup> between 43 and  $\sim 200$  eV/amu. The discrepancy in the slope for higher energies may be due to our neglect of other electronic capture channels. The ESS measurements of Burns *et al.*<sup>38</sup> suggest that capture into  $N^+(^3P^0, ^1D, ^3P)$  will become important above  $\sim 300$  eV/amu.

## 5 Conclusions

In this progress report, we have described our efforts to apply quantal MOCC techniques to the study of low energy multiply charged ion-molecule charge transfer. The present calculation, using potential curves for a collinear collision system over a range of  $H_2$  internuclear distances, has been shown to be consistent with the few available experimental data. Future work entails determining IOSA cross sections for a variety of orientations of the colliding species. This will necessitate the computation of the  $NH_2^+$  potential surfaces and coupling matrix elements for a range of  $\theta$ ,  $r$ , and  $R$ . Future studies will also include additional  $N^+$  capture channels for SEC and investigations of DEC and DiEC.

## Acknowledgements

The work of P.C.S. was performed at Oak Ridge National Laboratory which is managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under Contract DE-AC05-96OR22464. B.Z. acknowledges support from NSF Cooperative Agreement OSR-9353227.

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M98000393



Report Number (14) ORNL/CP--94781  
CONF-970710--  
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Publ. Date (11) 199709

Sponsor Code (18) DOE/ER NSF, XF

UC Category (19) UC-400 UC-000, DOE/ER

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