



Negative Ion Binding Energies in Complex Heavy Systems

Topical Review

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Abstract. We review briefly the recent progress in the determination of accurate and reliable electron affinities (EAs) of complex heavy systems with the view of assessing the reliability of the existing measured and/or calculated EAs of these systems. We demonstrate using slow electron collisions with complex heavy systems a novel and robust approach to the determination of reliable EAs from negative ion formation. From the Regge-pole calculated elastic total cross sections (TCSs), characterized by Ramsauer-Townsend (R-T) minima, shape resonances and dramatically sharp resonances manifesting anionic formation, we extract the anionic binding energies (BEs) for the ground, metastable and excited anionic states formed during the collisions. The ground state anionic BEs located at the absolute values of the R-T minima are identified with the systems' EAs. Results for various complex heavy systems, including fullerene molecules are compared with available measurements and calculations.

Keywords. Complex heavy systems; Electron affinity; Complex angular momentum; Negative ions; Anionic binding energies; Resonances

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1. Introduction

The determination of accurate and reliable electron affinity values of complex heavy systems, such as the lanthanide and actinide atoms, including the fullerene molecules is one of the most challenging problems in atomic and molecular physics, when exploring negative ion formation in low-energy electron scattering. And to date still continues to plague both experiments and

theory. Accurate and reliable atomic and molecular affinities are essential for understanding chemical reactions involving negative ions [1], whose importance and vast utility in terrestrial and stellar atmospheres as well as in device fabrication, drug delivery and organic solar cells are well-documented.

In the lanthanide and actinide atoms, in particular the presence of two or more open d- and f-subshell electrons presents formidable computational complexity when using conventional theoretical methods to calculate electron affinities (EAs) of complex heavy systems. Thus, recent years have witnessed the proliferation in the published literature of incorrect experimental and theoretical EAs for the lanthanide [2] and actinide [3] atoms as well as for atomic Nb. For the complex atoms such as Nb experiments have concentrated efforts mainly on the accuracy rather than on the reliability of the existing EAs. These reflect the difficulties in the theoretical understanding of the fundamental mechanism responsible for low-energy electron attachment in these systems leading to stable negative ion formation. Here we use our robust Regge pole methodology to explore negative ion formation in low-energy electron scattering from complex heavy systems through total cross sections (TCSs) calculations; their anionic ground state binding energies (BEs) are identified with the EAs. The methodology is appropriate since Regge poles are generalized bound states in the complex angular momentum (CAM) description of scattering. Its strength is that the calculations are based on a rigorous definition of resonances, viz. as singularities of the S-matrix.

This review paper has been motivated by the following:

- (1) In [2] it was concluded that both the measured and the calculated EAs for the lanthanide atoms Eu[4-8], Tb[9,10], Tm[11,12], Gd[5,10] and Nd[5,6,9], including the Nb[13-16] atom require reinterpretation. New recommended EA values for these atoms were presented.
- (2) For the fullerene molecules, C₂₀ through C₉₂ high quality measured EAs are available [17-32], but theoretical EAs are almost non-existent.
- (3) Very recently, the ground state anionic BEs, extracted from the Regge-pole calculated electron scattering TCSs were found to match excellently the measured EAs from C₂₀ through C₉₂ for the first time [33, 34]. The Regge pole methodology requires no assistance whatsoever from either experiment or other theory to achieve the remarkable results.
- (4) The low-energy electron elastic scattering TCSs for the complex heavy systems have been found to be characterized generally by Ramsauer-Townsend (R-T) minima, shape resonances (SRs) and dramatically sharp resonances manifesting ground, metastable and excited anionic formation during the collisions. Consequently, a robust theory is needed to guide the delineation and identification of the resultant resonance structures in the TCSs.
- (5) Very recently, electron scattering TCSs for the very complicated actinide atoms Th, Pa, U, Np and Pu were calculated [3]. It was concluded that the existing theoretical calculations tend to identify incorrectly the BEs of the resultant excited anionic states with the EAs of the investigated actinide atoms; this suggests a need for an unambiguous definition and determination of the EAs.

Recently, a theoretical breakthrough was achieved in low-energy electron scattering from complex heavy atoms and fullerene molecules through the use of the Regge pole, also known as the CAM methodology. The crucial electron-electron correlation effects and the vital core-polarization interaction have been identified as the major physical effects mostly responsible for electron attachment in low-energy electron scattering from complex heavy systems, leading to stable negative ion formation. Therefore, this report contrasts the results of the robust Regge pole methodology with those from measurements and calculations. The objective is to assess the reliability of the existing EA values and recommend new ones where necessary; this is particularly important for the experimentally difficult to handle radioactive actinide atoms.

2. Method of Calculation

For the near-threshold electron-neutral atom/fullerene collisions resulting in negative ion formation as resonances, we calculate the TCSs using the Mulholland formula [35]. In the form below, the TCS fully embeds the electron-electron correlation effects [36, 37] (atomic units are used throughout):

$$\sigma_{tot}(E) = 4\pi k^{-2} \int_0^{\infty} \text{Re}[1 - S(\lambda)] \lambda d\lambda - 8\pi^2 k^{-2} \sum_n \text{Im} \frac{\lambda_n \rho_n}{1 + \exp(-2\pi i \lambda_n)} + I(E). \quad (2.1)$$

In eq. (2.1) $S(\lambda)$ is the S -matrix, $k = \sqrt{2mE}$, m being the mass and E the impact energy, ρ_n is the residue of the S -matrix at the n th pole, λ_n and $I(E)$ contains the contributions from the integrals along the imaginary λ -axis; its contribution has been demonstrated to be negligible [5].

As in [38] here we consider the incident electron to interact with the atom/fullerene without consideration of the complicated details of the electronic structure of the system itself. Therefore, within the Thomas-Fermi theory, Felfli *et al.* [39] generated the robust ABF potential

$$U(r) = -\frac{Z}{r(1 + \alpha Z^{1/3} r)(1 + \beta Z^{2/3} r^2)}, \quad (2.2)$$

where Z is the nuclear charge, α and β are variation parameters. Note also that the ABF potential has the appropriate asymptotic behavior, *viz.* $\sim -1/(\alpha\beta r^4)$ and accounts properly for the polarization interaction at low energies. This potential, extensively studied [40], has five turning points and four poles connected by four cuts in the complex plane. The presence of the powers of Z as coefficients of r and r^2 in eq. (2.2) ensures that spherical and non-spherical atoms/fullerenes are correctly treated. The effective potential is considered here as a continuous function of the variables r and complex λ . The details of the numerical evaluations of the TCSs have been described in [37] and further details of the calculations may be found in [41].

The novelty of our approach lies in that the electron-electron correlation and core polarization interaction effects are accounted for adequately. Crucial in the CAM methods are the Regge trajectories, *viz.* $\text{Im} \lambda_n(E)$ versus $\text{Re} \lambda_n(E)$ ($\lambda_n(E)$ is the CAM) that probe electron attachment at the fundamental level near threshold, thereby allow the determination of reliable EAs. Thylwe [42], investigated Regge trajectories, using the ABF potential, and demonstrated that for Xe the Dirac Relativistic and non-Relativistic Regge trajectories yielded essentially the same $\text{Re} \lambda_n(E)$ when the $\text{Im} \lambda_n(E)$ was still very small. This clearly demonstrates the insignificant

difference between the Relativistic and non-Relativistic calculations at near threshold electron impact energies, if the appropriate physics is accounted for adequately as in this case.

The potential (2.2) has been used successfully with the appropriate values of α and β . It has been found that when the TCS as a function of β has a resonance [5], corresponding to the formation of a stable negative ion, this resonance is longest lived for a given value of the energy, which corresponds to the EA of the system (for ground state collisions) or the BE of the excited anion. This was found to be the case for all the systems, including fullerenes we have investigated thus far. This fixes the optimal value of “ β ” in eq. (2.2) when the optimum value of $\alpha = 0.2$.

The effective use of $Im \lambda \rightarrow 0$ is demonstrated in [5] and carefully explained in [43]. The physical interpretation of $Im \lambda$ is given in [44,45]. For a long lived resonance the lifetime $Im \lambda$ is small and the angular life $\Delta\theta$ is large. For a true bound state, negative E , $Im \lambda$ vanishes and the orbit becomes permanent. Obviously, in our calculations $Im \lambda$ is not identically zero, but small – this can be clearly seen in the figures; the long-lived resonances hardly have a width as opposed to shape resonances for instance (see also our paper ref. [5] for comparison).

3. Results

Figures 1 and 2 display our calculated TCSs for Au, C₆₀, Pu and C₁₃₂. These, typical for complex heavy systems, are characterized by R-T minima, SRs and dramatically sharp resonances manifesting negative ion formation during the collisions. The BEs presented in Table 1 for the various complex heavy systems were extracted from the positions of the very sharp resonances in the TCSs. Most importantly, the ground states anionic BEs are identified with the EAs and compared with the measured and/or calculated values. Indeed, the figures demonstrate the need for delineation and identification of the resonance structures to minimize misidentification of the various sharp peaks as explained in [2]. Suffice to state here that the ground, metastable and excited states anionic BEs of all the complex heavy systems were extracted from such TCSs as in Figures 1 and 2. As seen from Table 1, the Au and C₆₀ ground state anionic BEs match excellently the measured EAs. This is the reason for their choice as standards.

The TCSs for each system in the figures appear to be complicated. However, these TCSs are readily understood and interpreted if we focus on a single color-coded curve at a time since it represents scattering from different states resulting in negative ion formation; a ground, metastable and higher excited states. We first focus on the e-Au TCSs in Figure 1. We briefly explain the physics behind the ground state curve of Figure 1 (left panel); the explanation will be applicable to all the results presented in the figures. As the incident electron approaches the Au atom in its ground state closer, the atom becomes polarized, reaching maximum polarization manifested through the appearance of the first R-T minimum in the TCS at about 0.72 eV. With the increase in energy, the electron becomes trapped by the centrifugal barrier whose effect is seen through the appearance of the SR at about 1.33 eV. As the electron leaks out of the Au atom, the polarizability of Au leads to the creation of the second deep R-T minimum at 2.23 eV.

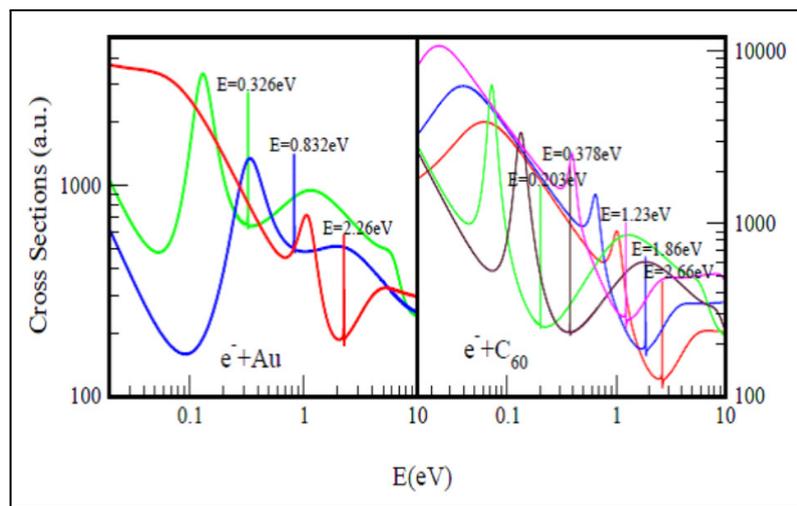


Figure 1. Total cross sections (a.u.) for atomic Au (left panel) and the C_{60} (right panel) are contrasted. For Au the red, blue and green curves represent TCSs for the ground, metastable and excited states, respectively. For C_{60} the red, blue and pink curves represent TCSs for the ground and the metastable states, respectively while the brown and green curves denote TCSs for the excited states. The very sharp resonances in both figures correspond to the Au^- and C_{60}^- negative ions formation during the collisions

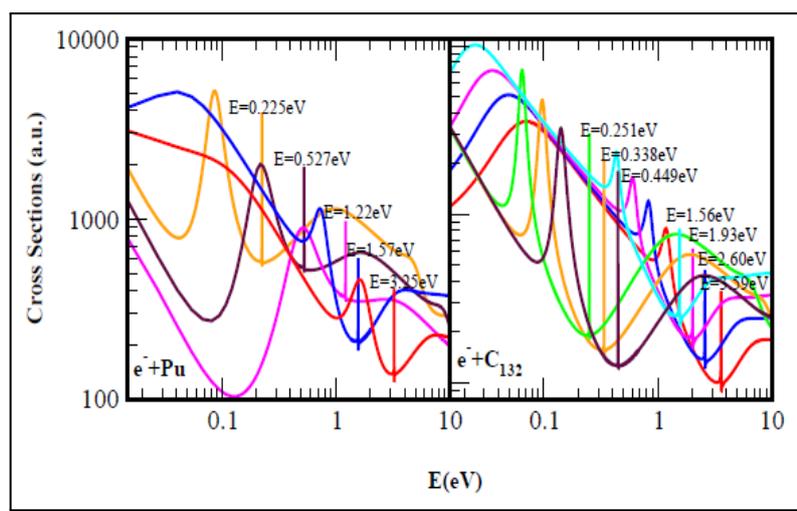


Figure 2. TCSs (a.u.) for atomic Pu (left panel) and the C_{132} (right panel) are contrasted. For Pu the red, blue and pink curves represent TCSs for the ground and metastable states, respectively while the brown and orange curves represent the excited states. For C_{132} the red, blue, pink and light blue curves represent TCSs for the ground and the metastable states, respectively. The brown, orange and green curves denote TCSs for the excited states. The very sharp resonances in both figures correspond to the Pu^- and C_{132}^- negative ions formation during the collisions

At the absolute minimum the long-lived ground state Au^- anion is formed; its BE is seen to be 2.26 eV, corresponding to the EA of atomic Au. At this R-T minimum the Au atom is transparent to the incident electron and the electron becomes attached to it forming the stable ground state Au^- anion. The electron spends many angular rotations about the Au atom as it decays. The long angular life time of the anionic ground state Au^- is determined by $1/Im \lambda \rightarrow \infty$,

since $Im \lambda \rightarrow 0$, see eq. (2.1). Indeed, the appearance of the R-T minima in the electron TCSs in Figure 1, demonstrating the crucial importance of electron correlation effects and polarization interaction, manifests that these effects have been accounted for adequately in our calculation, consistent with the conclusion in [46]. The rest of the curves in the figures can be analyzed similarly.

In Table 1 measured and/or calculated EAs for selected complex heavy systems are presented for comparison. What is important in the comparison is that consistent with the results for Au, Pt and C₆₀ the ground states BEs of the formed negative ions during the collisions correspond to the EAs. A glance at Table 1 allows for a quick assessment of the reliability of the existing experimental/theoretical EAs. The second and third columns in Table 1 represent respectively our ground states anionic BEs and the measured EAs. Indeed, for Au, Pt and C₆₀ outstanding agreement is realized between our BEs and the EAs, giving great credence to the ability of the Regge pole methodology to produce reliable EAs for complex heavy systems.

Table 1. Negative ion binding energies (BEs), in eV obtained from the TCSs for the complex heavy atoms and fullerene molecules (GRS, MS- n and EX- n ($n = 1, 2$) represent respectively ground, metastable and excited states. The experimental EAs, EXPT and the theoretical EAs, in eV are also presented. N/A denotes not available, table demonstrates the importance of determining the ground state BEs of the formed anions during the collisions; they yield the EAs for the complex heavysystems.)

System	BEs GRS	EAs EXPT	BEs MS-1	BEs MS-2	BEs EX-1	BEs EX-2	EAs Theory
Au	2.26	2.309[47] 2.301[48] 2.306[49]	0.832	-	0.326	-	2.262[50]
C60	2.66	2.666 [18] 2.683 [26] 2.650[24], 2.6835[17] 2.689 [25]	1.86	1.23	0.203	0.378	2.663[34] 2.57[71] 2.23[72] 2.63[73]
Nb	2.48	0.9174[13] 0.894[16]	0.902	-	0.356	-	0.82[14] 0.99[15]
La	2.26	0.47[51] >0.5[52]	0.478	-	0.115	-	0.478[5] 0.55[74]
Ce	2.42	0.955 [53] 0.65[54] 0.7[55] 0.57[56]	0.610	-	0.101	-	0.58[75] 0.660[57] 0.610[5]
Nd	1.88	>1.916[9]	-	-	0.162	-	0.167[6] 0.162[5]
Eu	2.63	0.116[4] 1.053[7]	1.13	-	0.116	-	0.116[5] 0.117[6] 1.08[8]
Gd	3.09	>0.1[10]	1.18	-	0.137	0.425	0.137[5]
Tb	3.04	>1.165[9] >0.1[10]	1.20	-	-	0.437	-
Dy	3.45	-	1.37	-	0.084	0.351	0.352[5] 0.063[6]
Tm	3.36	1.029[11]	1.02	-	0.274	-	0.027 - 0.136[12]
Yb	3.49	< 0.003[58] -0.02[60]	0.485	-	0.204	-	0.028[5] 0.036[59]
				-		-	

System	BEs GRS	EAs EXPT	BEs MS-1	BEs MS-2	BEs EX-1	BEs EX-2	EAs Theory
Pt	2.16	2.128[47] 2.125[48] 2.125[61] 2.123[62]	1.197	-	0.136	-	2.163[50]
At	2.51	N/A	0.918	-	0.292	-	2.51[63] 2.42[64] 2.81[65]
Th	3.09	N/A	1.36	-	0.549	0.905	0.368 [66] 0.368[67] 1.17[68]
Pa	2.98	N/A	1.49	-	0.395	0.874	0.222[69] 0.384[67] 0.55[68]
U	3.03	N/A	1.44	-	0.220	0.507	0.175[70] 0.373[67] 0.53[68]
Np	3.06	N/A	1.47	-	0.248	0.521	0.313[67] 0.48[68]
Pu	3.25	N/A	1.57	1.22	0.225	0.527	0.085[67] -0.50[68]
C20	2.72	2.250 [27] 2.70 [20] 2.600[29] 2.440[30]	1.48	-	0.466	-	-
C24	3.79	3.750 [29] 2.90 [28]	2.29	1.41	0.428	0.801	3.55[76]
C70	2.70	2.676 [18] 2.72[20] 2.765[19] 2.74[32]	1.77	1.27	0.230	0.364	-
C100	3.67	N/A	2.70	2.04	0.242	0.379	-
C132	3.59	N/A	2.60	1.93	0.251	0.338	-
C240	4.18	N/A	-	-	-	-	2.32[72] 3.81[77]

4. Conclusions

In this brief review we have surveyed low-energy electron scattering from complex heavy systems such as the fullerenes and the lanthanide and actinide atoms through the elastic TCSs calculations to assess the reliability of existing EAs. We found that all the TCSs are characterized by very sharp resonances manifesting anions formation during the collisions. From the energy positions of the anionic resonances we extracted their BEs with those for the anionic ground states being identified with the EAs of the investigated systems. For the fullerene molecules our extracted ground anionic BEs matched excellently the measured EAs. Significantly, for the lanthanide and actinide atoms, the measurements and/or calculations tend to identify incorrectly the BEs of the metastable/excited anionic states with the EAs. Indeed, the importance of the delineation and identification of the resonances in the electron collision TCSs are demonstrated by the Figures 1 and 2.

It is hoped that this review will provide an impetus to develop appropriate theoretical methods for the calculation of reliable EAs of complex heavy systems, such as the lanthanide and actinide atoms and the fullerene molecules to guide future measurements. The strength and beauty of the Regge pole methodology is that it requires no assistance whatsoever from either experiment or other theory to achieve the remarkable results.

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Competing Interests

The author declares that he has no competing interests.

Authors' Contributions

The author wrote, read and approved the final manuscript.

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