

Electron Collisions with Multielectron Atoms and Fullerene Molecules: Strong Polarisation Effects

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Abstract

Regge pole-calculated low-energy electron elastic total cross sections for multielectron atoms/fullerenes are characterised by ground, metastable and excited negative-ion formation, shape resonances and Ramsauer-Townsend minima. In this article, we demonstrate through the total cross sections for Eu, Au and At atoms and C₆₀ fullerene the sensitivity of stable negative-ion formation to the crucial core-polarisation potential. The energy positions of the dramatically sharp resonances corresponding to the binding energies of the formed anions during the collisions agree excellently with the measured electron affinities of the atoms and C₆₀. The sensitivity of Ramsauer-Townsend minima and shape resonances to the electronic structure and dynamics of Bk and Cf permits their first ever use as novel validation of the experimental observation that Cf is indeed a transitional element in the actinide series. Their electron affinities are also calculated.

Keywords: Multielectron atoms, electron correlation, core-polarisation, cross sections, electron affinities, fullerene molecules, negative ions, Regge poles

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1 Introduction

The measured electron affinities (EAs) of Au, At and C_{60} correspond to the Regge pole-calculated negative ion binding energies (BEs) when the incident electron is attached in the ground state of the formed negative ion during the collision. For most of the actinide and the lanthanide atoms, the measured and the calculated EAs have been identified with the Regge pole BEs when the incident electron is attached in an excited state of the negative ion formed during the collision [1]. The actinide atoms, owing to their highly radioactive nature, are difficult to handle experimentally. Consequently, only the EAs of Th and U have been measured thus far. However, theoretical EAs are available for most of the actinide atoms. Unfortunately, these EAs are riddled with uncertainties and are therefore also difficult to understand and interpret.

The recent experiment [2] using only a single nanogram of the highly radioactive Bk and Cf atoms characterised their structure and dynamics, and concluded that indeed Cf is a transitional element in the actinide series. The observation [2] has been validated through the sensitivity of the Regge pole-calculated Ramsauer-Townsend (R-T) minima and shape resonances (SRs) in the polarisation induced metastable total cross sections (TCSs) of Bk and Cf, that is, the deep R-T minimum characterising the Bk metastable TCS flips over to an SR very close to threshold in the metastable TCS of the Cf atom. This experimental breakthrough [2], the recent first ever measurement of the EA of the highly radioactive At [3] and the recent measurements of the EAs of Th [4] and U [5] [6] represent significant advances in the measurements of the highly radioactive elements. More such measurements of other radioactive atoms can be expected in the near future. Consequently, a fundamental understanding of the underlying mechanism of negative ion formation is vital for reliable theoretical predictions to guide the EA measurements. This explains the motivation for the current investigation. In addition, Berkelium has been used in the synthesis of heavier elements such as Tennessine, while Californium, a very strong neutron emitter, is used *inter alia* in identifying gold and silver ores as well as in detecting metal fatigue and stress in airplanes.

2 Method of Calculation

The existing very sophisticated theoretical methods developed in atomic and molecular physics were tasked with reproducing experimental results, such as the EAs of multielectron atoms with high accuracies. Indeed, in most cases, they provided agreement with experiment, but did very little to unravel and elucidate the intricate details and the precise description of the nature of the different physical effects that are important to a particular process. Importantly, they also lacked the predictive power. In the solutions of scattering problems using standard quantum mechanical approaches, the desired solutions are often expressed as a partial-wave (PW) sum over the orbital (or total) angular momentum quantum number. This notoriously very slowly convergent PW expansion may contain hundreds, if not thousands, of terms. The obtained EAs using these methods are often riddled with uncertainties and are therefore difficult to interpret.

However, in the complex angular momentum (CAM) description of scattering, involving Regge poles calculations [7], this slowly convergent PW series becomes a more rapidly converging series. This leads us to the concept of Regge poles: they are simply generalised bound states, namely, solutions of the Schrödinger equation when the energy E is real, positive and the angular momentum λ is complex. Mathematically, Regge poles, singularities of the S-matrix, rigorously define resonances [8], [9] and in the physical sheets of the complex plane, they correspond to bound states [10]. The Regge poles formed during low-energy electron elastic scattering become stable bound states [11]. In the near-threshold electron–atom/fullerene molecule collision resulting in negative ion formation as resonances, the calculation of the electron elastic TCSs exploits the rigorous Regge pole method through the Mulholland formula [12]. This formula converts the infinite discrete sum into a background integral plus the contribution from a few poles to the scattering process under consideration.

Indeed, the method requires no a priori knowledge of the experimental or any other theoretical data as inputs, hence, its predictive nature. Electron–electron correlations and core-polarisation interactions are both crucial for the existence and stability of most negative ions. The former effects are embedded in the Mulholland formula as implemented in [13], [14] for the TCSs, while the latter interactions are incorporated through the well-investigated Thomas–Fermi type model potential [15], [16]. The Mulholland formula [12] used here is of the form [13], [14] (atomic units are used throughout):

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

In Equation (1), $S(\lambda)$ is the S-matrix, $k = \sqrt{2mE}$, $m = 1$ 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 (λ is the CAM); its contribution has been demonstrated to be negligible [17].

As in [18], we consider the incident electron to interact with the complex heavy system without consideration of the complicated details of the electronic structure of the system itself. Thus, the robust Avdonina–Belov–Felfli potential [19], which embeds the vital core–polarisation interaction, is used:

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

In Equation (2), Z is the nuclear charge, α and β are variation parameters. For small r , the potential describes Coulomb attraction between an electron and a nucleus, $U(r) \sim -Z/r$, while at large distances it has the appropriate asymptotic behaviour, namely, $\sim -1/(\alpha\beta r^4)$ and accounts properly for the polarisation interaction at low

energies. For an electron, the source of the bound states generating the Regge trajectories, also important quantities calculated in CAM theories, is the attractive Coulomb well it experiences near the nucleus. The addition of the centrifugal term to the well “squeezes” these states into the continuum [14], [20]. For larger λ , the effective potential develops a barrier. Consequently, a bound state crossing the threshold energy $E = 0$ in this region may become an excited state or a long-lived metastable state. As a result, the highest “bound state” formed during the collision is identified with the highest excited state, here labelled as EXT-1 (see Table 1). As E increases from zero, the second excited state may form with the anionic BE labelled, EXT-2. For the metastable states, similar labelling is used as MS-1, MS-2, etc. However, it should be noted here that the metastable states are labelled relative to the anionic ground state and that $1/(\text{Im } \lambda)$ determines the angular life of a resonance [7], [9].

The strength of this extensively studied potential, Equation (2) [15], [16], lies in that it 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 Equation (2) ensures that spherical and non-spherical atoms and fullerenes are correctly treated. Small and large systems are also appropriately treated. The effective potential $V(r) = U(r) + \lambda(\lambda + 1)/(2r^2)$ is considered here a continuous function of the variables r and complex λ . Importantly, our choice of the potential, Equation (2), is adequate as long as our investigation is confined to the near-threshold energy regime, where the elastic TCS is less sensitive to short-range interactions and is determined mostly by the polarisation tail. The numerical calculations of the TCSs, limited to the near-threshold energy region, that is, below any excitation thresholds to avoid their effects, the pole positions and the residues are carried out by solving the Schrödinger equation as described in [14], see also [21]. The parameters “ α ” and “ β ” of the potential in Equation (2) are varied, and with the optimal value of $\alpha = 0.2$, the β -parameter is further varied carefully until the dramatically sharp resonance appears in the TCS [17]. This is indicative of stable negative ion formation during the collision and the energy position matches with the measured EA of the atom/fullerene molecule (see, for example, the Au and C₆₀ fullerene TCSs in [22]). This has been found to be the case in all the atoms and fullerenes investigated thus far.

Here the colliding partners (electron-atom/fullerene) are assumed to form a long-lived intermediate complex, manifesting as a sufficiently narrow resonance that rotates as it decays at zero scattering angle to preserve the total angular momentum. If the complex has a long angular life, namely $\text{Im } \lambda \ll 1$, it will return to forward scattering many times. For the resonance to contribute to the TCS two resonance conditions must be satisfied: (1) Regge trajectory, namely $\text{Im } \lambda$ versus $\text{Re } \lambda$ stays close to the real axis, and (2) real part of the Regge pole is close to an integer.

3 Results

In this section we first discuss the vital importance of the Regge trajectories in the determination of rigorous negative ion BEs during collisions as well as demonstrate the

sensitivity of the Regge pole-calculated BEs to the parameters “ α ” and “ β ” of the potential in Equation (2), essentially to the polarisation interaction, using as examples the Eu, Au and At atoms. Then the TCSs for the actinide atoms Bk and Cf are presented whence the rigorous EAs are extracted.

3.1 Regge Trajectories

Thylwe [23] carried out one of the most significant and revealing investigations of the importance of Regge trajectories, namely, $\text{Im } \lambda(E)$ versus $\text{Re } \lambda(E)$ (the explicit energy dependence is inserted here) in low-energy electron collisions with multielectron atoms using the potential in Equation (2). For the Xe atom, Regge trajectories were explored using both the Dirac relativistic and non-relativistic methods. It was found that near the threshold energy region both calculations yielded essentially the same $\text{Re } \lambda(E)$ when the $\text{Im } \lambda(E)$ was still very small (see Figure 2 of [23]). This implied the insignificant difference between the relativistic and non-relativistic calculations when the electron impact energy E was still small, which is the condition of our calculations here. For the less studied C_{60} fullerene molecule, here we investigated the Regge trajectories for the ground state ($\text{Re } \lambda(E) = 5$) and the shape resonance ($\text{Re } \lambda(E) = 3$). Clearly seen from Figure 1(a) is that the Regge trajectory corresponding to $\text{Im } \lambda \ll 1$ stays close to the real axis and has a pole energy value of 2.66 eV and $\text{Re } \lambda(E) = 5$. This energy, 2.66 eV, determines the ground state BE of the C_{60} negative ion formed during the collision, and hence is identified with the EA of C_{60} [24] as seen from Table 1. In Figure 1(b), the Regge trajectory of the pole responsible for the shape resonance at $E = 1.02$ eV with $\text{Re } \lambda(E) = 3$ corresponds to $\text{Im } \lambda(E)$ that is significantly larger than that for the $\text{Re } \lambda(E) = 5$, as expected (see also [17]).

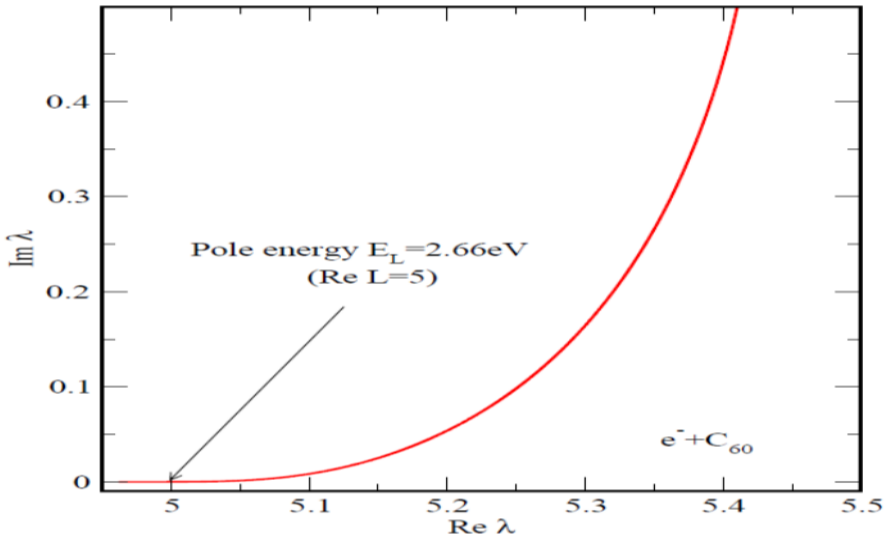


Figure 1(a). Regge trajectory of the pole responsible for the ground state energy $E = 2.66$ eV with $\text{Re } \lambda(E) = 5$ for C_{60}

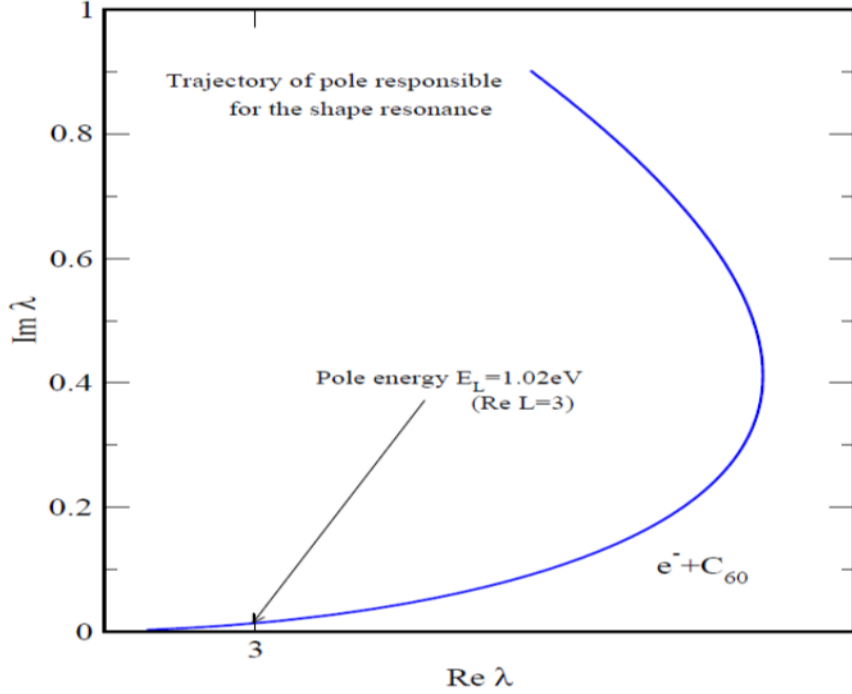


Figure 1(b). Regge trajectory of the pole responsible for the shape resonance at $E = 1.02$ eV with $\text{Re } \lambda(E) = 3$ for C_{60}

3.2 Polarisation Interaction Effect on the Calculation of the Binding Energies

Figures 2, 3 and 4 demonstrate the variation of the TCSs for the atoms Eu, Au and At, respectively, with the β -parameter of Equation (2) when the optimal $\alpha = 0.2$. Figure 2 shows the variation of the TCS for Eu with E, demonstrating its sensitivity to the values of β (b is used in Figure 2 for convenience) when the optimal value of $\alpha = 0.2$. Beginning with the value of $b = 0.0370$ (blue curve), the TCS exhibits no stable negative ion formation until $b = 0.0375$ when the sharp red line appears, indicative of a long-lived negative ion formation. As b increases beyond 0.0375 to $b = 0.0376$ (green curve), there is no stable negative ion formation supported by the potential. The energy value, namely the BE at the red line is 0.116 eV [17] and is in outstanding agreement with the measured EA value of 0.116 eV [25] as well as the MCDF-RCI calculated value of 0.117 eV [26]. We stress here that below and beyond the $b = 0.0375$ value the potential supports no stable negative ions. It is also revealing to check the $\text{Im } \lambda$ in [17].

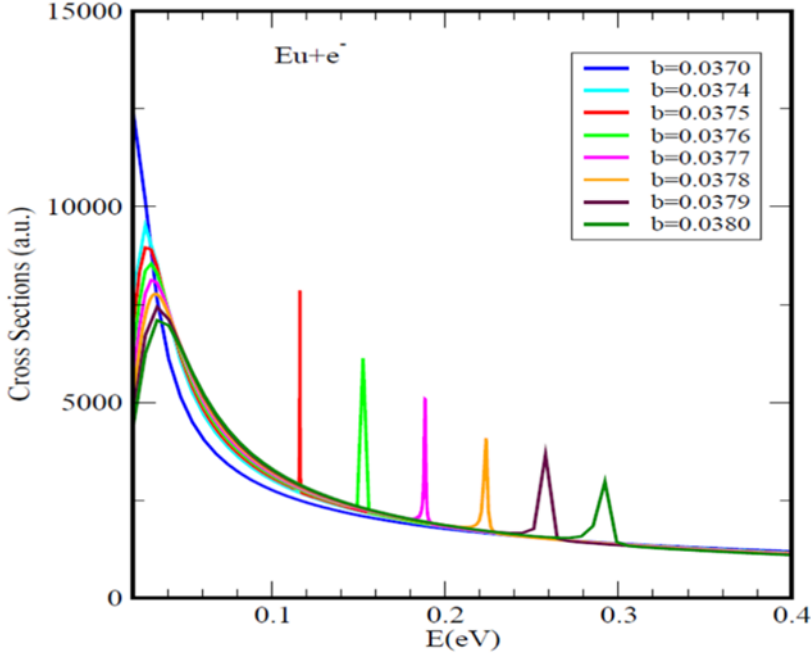


Figure 2. Electron elastic scattering TCS (a.u.) versus E (eV) for atomic Eu, demonstrating the sensitivity of the BE (electron affinity) to the “ β ” parameter of the polarisation potential, when the optimal value of $\alpha = 0.2$. (b is used for the values of β in the figure)

Figure 3 displays the variation of the TCS for Au with the β -parameter (b is used in Figure 3 for convenience). Similarly, as in Figure 2, a stable negative ion of Au is formed when $b = 0.0360$ (sharp green line). The BE corresponding to this b value is 2.263 eV; it is very close to the measured EAs of Au [27], [28], [29] and to the EA calculated using the most sophisticated theoretical method to date [30]. Indeed, the excellent agreement with the measured EAs of Au demonstrates that the Regge pole analysis is the appropriate method to use for calculating reliable EAs of heavy multielectron atoms. The results for the highly radioactive At atom are displayed in Figure 4. Of interest with the At results is that with $b = 0.0420$ we obtained the BE of 2.51 eV [31] close to the then known calculated EA of 2.80 eV [32]. Around the same time, the EA value of 2.42 eV was calculated using the MCDF method [33]. After the measured EA of 2.416 eV [3] was published, we carefully re-examined the value of the β -parameter we used above. The sharpest resonance occurred when $\beta = 0.04195$, which yielded the BE of 2.42 eV in outstanding agreement with the measured and the recent theoretical EAs [34], [35], [36]. Note that when β is greater than or less than 0.04195 there are no stable negative ions formed during the collision.

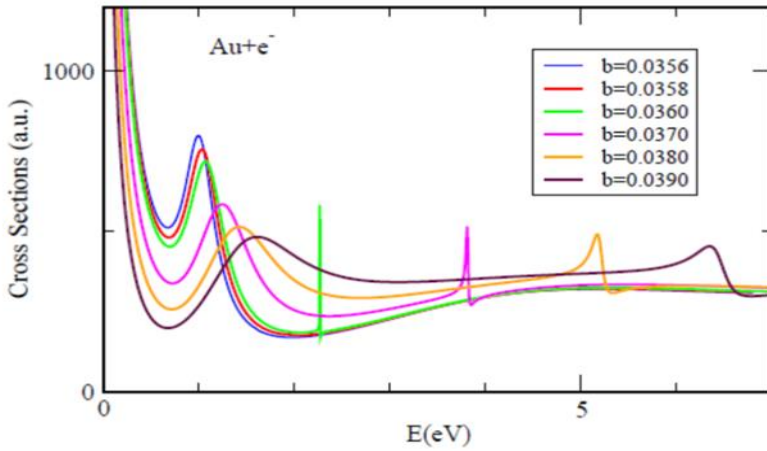


Figure 3. Electron elastic scattering TCS (a.u.) versus E (eV) for atomic Au, demonstrating the sensitivity of the BE (electron affinity) to the “ β ” parameter of the polarisation potential, when the optimal value of $\alpha = 0.2$. (b is used for the values of β in the figure)

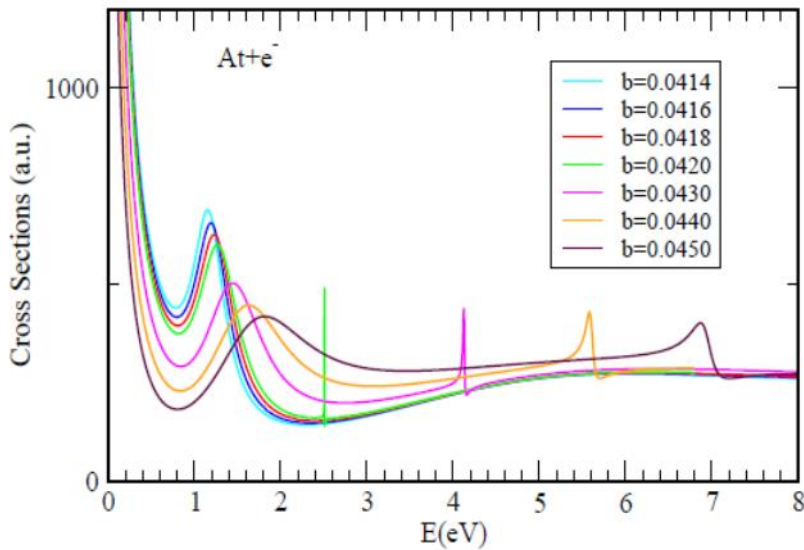


Figure 4. Electron elastic scattering TCS (a.u.) versus E (eV) for atomic At, demonstrating the sensitivity of the BE (electron affinity) to the “ β ” parameter of the polarisation potential, when the optimal value of $\alpha = 0.2$. (b is used for the values of β in the figure)

Indeed, the outstanding agreement between the Regge pole BEs and the measured EAs of Eu, Au and At atoms as well as of the C₆₀ [37], [38], [39] and other fullerenes [24] gives great credence to the Regge pole analysis to produce rigorous and unambiguous BEs, requiring no assistance whatsoever from either experiment or any other theory to achieve the remarkable feat. It also strengthens our interpretation of the EAs of these complex systems, namely as corresponding to the ground state BEs of the formed negative ions during the collisions. Metastable and excited states BEs are also calculated similarly.

3.3 On the Relativistic Effects in Electron Affinity Calculation Using Regge Pole Analysis

Most of the sophisticated theoretical calculations of the EAs of multielectron atoms include relativistic effects at various levels of approximations. See, for example, their comparisons in the calculation of the EA of the highly radioactive At atom in [34]. Of particular interest here is that a stringent test of the nonrelativistic Regge pole analysis is exhibited when the calculated BE (0.116 eV) [17] of Eu ($Z = 63$) is compared with the EA value of 0.117 eV calculated using the MCDF-RCI method [26] and with the measured EA (0.116 eV) [25]. Indeed, the agreement between the theoretical and the experimental EA values is outstanding. Incidentally, the theoretical values [17], [26] were obtained almost a decade before the measurement was carried out, but certainly after the measurement [40].

The relativistic couple cluster method with variational quantum electrodynamics [30] achieved an impressive EA value for the Au atom, which is in outstanding agreement with the measured EAs of Au [27], [28], [29]. This EA value that is challenging to calculate is also in excellent agreement with the Regge pole-calculated BE value for Au, obtained in 2008 [41] (see also Table 1 for comparisons with other EAs [42], [43]). For the highly radioactive At atom, the recently measured EA [3], which employed the coupled cluster method, agreed excellently with the Regge pole-calculated BE and the EAs from various sophisticated theoretical calculations, including the multiconfiguration Dirac–Hartree–Fock values [33]–[36] (see Table 1 for comparisons). Furthermore, in [34] and [35] extensive comparisons among various sophisticated theoretical EAs have been carried out as well. Indeed, for the Eu, Au and At atoms as well as the C₆₀ and the C₇₀ [38], [44], [45] fullerenes, the Regge pole analysis requires no a priori knowledge of the experimental or any other theoretical data as inputs to achieve the remarkable agreement. These results give great credence to the predictive power of the Regge pole analysis. The two differing calculated EA values of C₇₀ by the same authors [46], simply demonstrate the great challenge facing theory.

3.4 Rigorous Negative Ion Binding Energies for Bk and Cf Atoms

The recent experiment [2] used only a single nanogram of Bk and Cf atoms and identified a weak spin-orbit-coupling in Bk while a jj coupling scheme described Cf. It concluded that these observations strengthen Cf as a transitional element in the actinide

series. The sensitivity of the Regge pole-calculated R-T minima and SRs in the polarisation-induced metastable TCSs of Bk and Cf has been exploited and used to validate the observation [2] through the flipping over of the near threshold deep R-T minimum in the Bk TCSs to an SR that is very close to threshold in the metastable TCS of the Cf atom (see Figure 5). Since there are no measured EAs for these elements and the existing theoretical EAs are ambiguous and difficult to understand (see Table 1), here we have reproduced our TCSs of the Bk and Cf atoms, taken from [1] with minor modification, to facilitate our discussion and guide both measurements and calculations of their EAs by producing robust values. It must be emphasised here that these EAs are challenging to calculate [47], [48] and to measure, manifested through the absence of their measured EAs (see Table 1). Also, the presence in Table 1 of only a few theoretical EAs of the C_{60} fullerene [24], [49], [50] is indicative of the difficulty of studying theoretically even this relatively simple fullerene, let alone the other fullerenes [24].

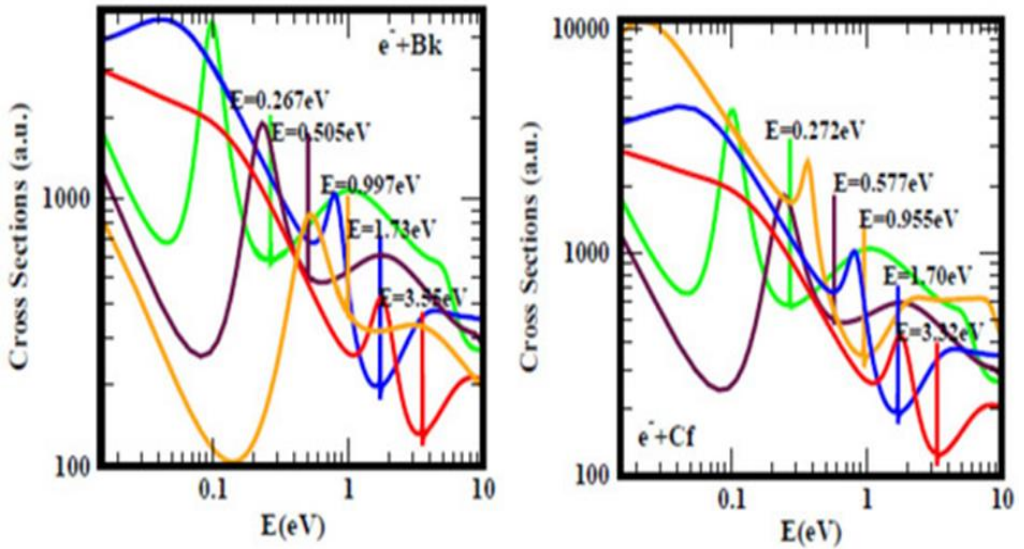


Figure 5. TCSs (a.u.) for atomic Bk (left panel) and Cf (right panel) are contrasted. For both Bk and Cf, the red, blue and orange curves represent TCSs for the ground and the metastable states, respectively, while the brown and the green curves correspond to excited state TCSs. The dramatically sharp resonances in the TCSs of both figures correspond to Bk- and Cf-negative ions formed during the collisions. The near-threshold deep R-T minimum in the polarisation-induced Bk TCS flips over here, since it first appeared in the Pu TCSs, to an SR that is very close to threshold in the Cf TCS.

Figure 5 shows that the Regge pole-calculated electron elastic TCSs, calculated as in Section 3.2 for both Bk and Cf, are characterised generally by dramatically sharp resonances, representing ground, metastable and excited negative ion formation, SRs and R-T minima. They also exhibit fullerene molecular behaviour near threshold

through the green curves [51]. The energy positions of the sharp resonances correspond to the anionic BEs of the formed negative ions during the electron collisions. In addition, a polarisation-induced metastable TCS with a deep R-T minimum is identified in the Bk TCSs. However, in the Cf TCSs, this R-T minimum appears as an SR very close to threshold. These peculiar tunable behaviours in the TCSs of these large actinide atoms are attributed to the size effects and orbital collapse, having a significant impact on the polarisation interaction in these atoms.

TABLE 1. Negative-ion BEs and ground states R-T minima, all in eV, extracted from the Regge pole-calculated TCSs of the atoms and the fullerene molecules C_{60} and C_{70}

System	BEs	BEs	BEs	EAs	BEs	BEs	R-T	BEs/EAs
Z	GRS	MS-1	MS-2	EXPT	EXT-1	EXT-2	GRS	Theory
Au 79	2.26	0.832	–	2.309[27] 2.301[28] 2.306[29]	0.326	–	2.24	2.313[30] 2.263[41] 2.50[42] 2.19[43]
At 85	2.42	0.918	0.412	2.416[3]	0.115	0.292	2.43	2.42[33] 2.38[34] 2.412[35] 2.45 [36]
Eu 63	2.63	1.08	–	0.116[25] 1.053[40]	0.116	–	2.62	0.117[26] 0.116[17]
C_{60}	2.66	1.86	1.23	2.684[37] 2.666[38] 2.689[39]	0.203	0.378	2.67	2.663[24] 2.57[49] 2.63[50]
C_{70}	2.70	1.77	1.27	2.676[38] 2.72[44] 2.74[45]	0.230	0.384	2.72	3.35[46] 2.83[46]
Bk 97	3.55	1.73	0.997	N/A	0.267	0.505	3.56	0.031[47] –0.276[48] –0.503[48]
Cf 98	3.32	1.70	0.955	N/A	0.272	0.577	3.34	–0.010[47] 0.018[47] –0.777[48] –1.013[48]

Note: They are compared with the measured EAs in eV. GRS, MS- n and EXT- n ($n = 1, 2$) denote respectively ground, metastable and excited states. Experimental EAs, EXPT and theoretical EAs are also included.

The characteristic R-T minima, also observed in the Dirac R-matrix calculated low-energy electron TCSs for the heavy alkali-metal atoms Rb, Cs and Fr [52], reflect the polarisation of the atomic core by the scattered electron [53]. Here, the R-T minima, important, inter alia, in understanding sympathetic cooling and cold molecules production from natural fermions [54], manifest that the important polarisation interaction has been accounted for adequately by our calculation consistent with the conclusion in [53]. Low-energy electron scattering deposits energy and induces chemical transitions through the mechanism of temporary negative ion formation as resonances [55]. Shape-resonance formation in low-energy electron collisions with atoms has been used to interpret electron-induced chemical processes resulting in

negative ion production [56]. The existence of a significant peak in the low-energy electron-atom scattering cross section manifests negative ion formation as a resonance [57]. As seen in Figure 5, this facilitates the unambiguous identification of negative ion formation considerably.

4 Concluding Remarks

We have investigated core-polarisation effects in low-energy electron collisions with multielectron atoms and fullerene molecules to assess their vital importance in stable negative ion formation. We found that in electron $-C_{60}$ collision, when E is still small and $\text{Im } \lambda \ll 1$, the obtained ground state BE of the C_{60}^- anion formed during the collision corresponds to the EA of C_{60} in excellent agreement with the measured EAs. This conclusion is also valid for the fullerenes from C_{20} through C_{92} [24]. We have also demonstrated using the atoms Eu, Au and At that their anionic BEs are very sensitive to the polarisation interaction potential. The optimal values of the α and β parameters of Equation (2) yield the anionic BEs corresponding to the measured EAs. In addition, the EAs obtained from relativistic calculations yield essentially the same BEs as the Regge pole-calculated values since the Regge pole analysis embodies the vital physics responsible for stable negative ion formation in low-energy electron scattering. It should be noted, however, that for both the Bk and Cf atoms, the calculated EAs using sophisticated methods do not make sense at all (see Table 1).

For the structurally complicated large Bk and Cf actinide atoms, the calculated TCSs are found to be characterised by well-delineated ground, metastable and excited negative ion formation, yielding their anionic BEs. And these have been used to assess the meaning of the existing theoretical EAs with the conclusion that those EAs are meaningless (see Table 1). We have also used the sensitivity of the R-T minima and the SRs of the polarisation-induced TCSs of Bk and Cf atoms to validate the recent experimental observation [2], thereby providing novel use of the R-T minima and SRs for the first time in this context. Finally, the doubly charged negative ions of the actinide atoms are expected to provide novel dynamic tunable catalysts as demonstrated in water oxidation into peroxide with Si^{2-} , Pu^{2-} , Pa^{2-} and Sn^{2-} being the best catalysts [58]. Thus, the radioactive elements usher in new application opportunities. Indeed, the great strength of the Regge pole analysis in understanding low-energy electron collisions with complex multielectron systems is through negative-ion formation, demonstrated through the extraction from the TCSs of rigorous and unambiguous negative-ion BEs, without any experimental or other theoretical assistance.

5 Acknowledgements

This research was supported by the Division of Chemical Sciences, Geosciences and Biosciences, the Office of Basic Energy Sciences, Office of Energy Research of the United States Department of Energy (U.S. DOE). The computing facilities of the National Energy Research Scientific Computing Center, also funded by the U.S. DOE, are greatly appreciated. We also thank Dr Kelvin Suggs for valuable discussions.

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