Resonances in low-energy electron elastic scattering from Fullerenes

Zineb Felfli[†] [1] **and Alfred Msezane**[†] [2]

[†] Department of Physics and CTSPS, Clark Atlanta University, Atlanta, Georgia 30314, USA

Synopsis The benchmarked Regge-pole method on the calculated low-energy electron elastic scattering total cross section (TCS) for C_{60} through the measured electron affinity (EA) [1,2] is used to calculate TCSs for selected fullerenes, from C_{54} through C_{240} in the electron impact energy range $0.02 \leq E \leq 10.0$ eV. From the characteristic dramatically sharp resonances representing long-lived ground state fullerene negative ion formation we extracted the binding energies (BEs) and compared them with the measured EAs, obtaining outstanding agreement.

The EA provides a stringent test of theory when the calculated and measured EAs are compared. A strong motivation for the fundamental investigations of low-energy electron elastic scattering from the selected fullerenes is the availability of high quality measured EAs [1-7]. The Regge pole calculated TCSs are found to be characterized generally by Ramsauer–Townsend (R-T) minima, shape resonances and dramatically sharp resonances manifesting stable negative ion formation. The extracted BEs for the resultant anions agree excellently with the measured EAs of the considered fullerenes giving great credence to the Regge pole method.

Table 1 displays the outstanding capability of the Regge pole method to calculate BEs of fullerene anions over a wide range of fullerenes. The method can also be used for complex atoms Fig. 1 displays the typical TCSs for electron-C_{76} scattering, exhibiting rich resonances.

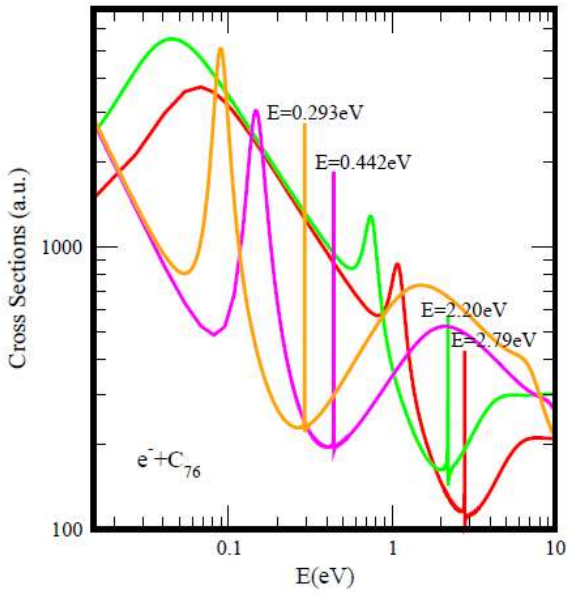

Fig. 1: TCSs for electron- C_{76} scattering.

Table 1: Comparison between the measured EAs (eV) and the present BEs (eV) for the investigated fullerenes, C_{54} through C_{240}.

System	EA-Expt. (eV)	BE-Present (eV)
C_{60}	2.666±0.001[2] 2.6835±0.0006[1]	2.66
C_{70}	2.72±0.05[4] 2.676±0.001 [2] 2.765(0.01)[3]	2.70
C_{74}	3.28±0.07[4] 3.28±0.07 [5]	3.21
C_{76}	2.88 ± 0.05[4] 2.89±0.05[5]	2.79
C_{78}	3.01±0.07[4] 3.10±0.06[5]; 3.10±0.01[6]	2.98
C_{54}	--	3.14
C_{80}	3.17 ± 0.06[4] 3.17±0.06 [5]	3.28
C_{82}	3.14±0.06[4] 3.14±0.06[5]	3.15
C_{84}	3.05±0.08[4] 3.14(6)[5]; 3.185±0.01[6] 3.16[7]	2.94
C_{86}	≥ 3.0 [4]	2.92
C_{90}	≥ 3.0 [4]	3.06
C_{92}	≥ 3.0 [4]	3.09
C_{180}		2.54
C_{240}		2.41

Research supported by U.S. DOE, OBES, OS

References

[1] D.-L. Huang *et al*. 2014 *J. Chem. Phys* **140** 224315
[2] C. Brink *et al.* 1995 *Chem. Phys. Lett.* **233** 52
[3] X. B. Wang *et al* 2006 *Phys Rev. Lett.* **96** 143002
[4] O. V. Boltalina *et al.* 1993 *J. Rapid Commun. Mass. Spectrom.* **7** 1009
[5] O. V. Boltalina *et al.* 1996 *Chem. Phys. Lett.* **256** 253
[6] X.–B. Wang *et al* 2007 *J. Phys. Chem. C* **111** 17684
[7] O. V. Boltalina *et al* 1997 *J. Phys. Chem. A* **101** 9561

[1] E-mail: zfelfli@cau.edu

[2] E-mail: amsezane@cau.edu