New insights in low-energy electron-fullerene interactions

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Synopsis Regge pole calculated low-energy electron scattering total cross sections (TCSs) for ground and first excited states of fullerenes are generally robust; for C_{20} they resemble those of atomic Au. Here we explore the variation of R, the ratio of second to first Ramsauer-Townsend minima of excited states TCSs, from C_{20} through C_{70} . We find that for C_{20} R is close to that for Au (> 1.) while for C_{24} R is about unity. For C_{70} R is less than 0.5 demonstrating strong departure from atomic behavior due to significant polarization interaction in C_{70} ; which also induces long-lived metastable anions in C_{70} .

The discovery of the now most studied C_{60} fullerene [1] inspired vigorous searches for new fullerenes, leading to the discovery of the smallest fullerene thought to exist, C_{20} . Its electron affinity (EA) was measured to be 2.25 eV [2]. Other small fullerenes of interest here are C_{24} , C_{26} , C_{28} and C_{44} , some of which have measured EAs available.

This investigation has been motivated by: 1) Amusia concluded that fullerenes can be viewed as "big atoms" [3]; 2) Rich resonances have been observed to characterize low-energy electron-fullerene interactions; 3) In [4] the Regge pole calculated low-energy electron elastic total cross sections (TCSs) for ground states C₆₀ through C_{92} were found to be characterized by dramatically sharp resonances located at the second Ramsauer-Townsend (R-T) minima of their TCSs. The energy positions of these sharp resonances were generally in outstanding agreement with the measured EAs for the investigated fullerenes and 4) The calculated TCSs revealed polarization induced long-lived metastable fullerene anions [4].

The departure from atomic behavior is studied through the ratio R focusing on the green curve of TCSs for C_{20} through C_{70} . In the Fig. the first R-T minima for both C_{20} and Au are lower than the second, indicative of atomic behavior. For C_{26} , R is about unity and for C_{70} it is < 0.5, demonstrating complete departure and conversion of the 0.466 eV resonance to a longlived metastable anion in C_{70} .

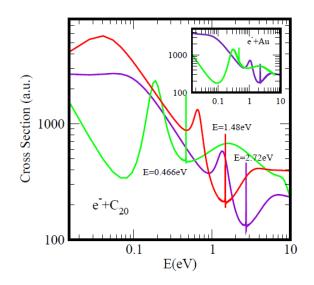


Figure 1: Total cross sections (a.u.) for electron elastic scattering versus E (eV) for C_{20} . The purple, pink and green curves represent results for the ground, induced metastable and first excited states, respectively; the insert represents TCSs for atomic Au. The dramatically sharp resonances correspond to fullerene anions formation during the collisions.

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References

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