Negative ions formation in fullerenes and heavy complex atoms

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Synopsis *Our robust Regge pole methodology is used to explore negative ion formation in low-energy electron elastic scattering from C_n (n=20 to 240) and selected heavy atoms through the total cross sections (TCSs) calculation. All the TCSs are found to be characterized by dramatically sharp resonances manifesting stable anionic formation during the collisions. The energy positions of the anionic ground states resonances are compared with the measured electron affinities*

Recently, a theoretical breakthrough was achieved in low-energy electron scattering from fullerenes through our robust Regge pole methodology [1], whe-rein is fully embedded the electron-electron correlations and the vital core-polarization interaction. Entirely new in the field of cluster/fullerene colli-sions, the Regge pole methodology was benchmarked on the measured electron affinities (EAs) of C_{60} and C_{70} fullerenes [2, 3].

The unprecedented accomplishments of the Regge pole methodology in low-energy electron elastic scattering are demonstrated in the following:

Ground state fullerene negative ion formation: The Regge pole methodology has been used to calculate ground state TCSs for selected fullerenes, from C_{54} through C_{240}. Our energy positions of the very sharp anionic resonances in the TCSs and the mea-sured EAs [2-4] matched excellently.

Long-lived metastable anions in fullerene mole-cules C_{60} to C_{92}: A strong motivation for the exploration is the availability of high quality measured EAs for the fullerenes from C_{60} through C_{92} [2-4] and the experimental observation that electron scattering cross sections from fullerenes are characterized by long lived metastable anionic formation [5]. Indeed, the TCSs are characterized by sharp resonances manifesting both ground and metastable anionic formation. Importantly, the metastable anionic states could be mistaken for the ground state anions and the impact of the size is drastic as the fullerene size changes from C_{76} through C_{82} to C_{92}; it induces additional metastable resonances in TCSs.

New insights in low-energy electron-fullerene interactions: Additional to producing first time anions in C_n (n=20, 24, 26, 28, 44, 70, 92 and 112) through low-energy electron scattering TCSs, here we also investigated the size-effect through the induced metastable resonances as the fullerene size varied from C_{20} through C_{112}. The C_{20} TCSs exhibit atomic behavior consistent with the view [6] while the C_{112} TCSs demonstrate strong departure from atomic behavior due to the size effect. Surprisingly, the small C_{24} has the largest EA, 3.79 eV among the
investigated fullerenes. It is therefore suitable for use in organic solar cells to counter the rate of irreversible polymer photobleaching in blend films (polymer: fullerene) and to resist fullerene degradation by the photo-oxidation mechanism [7]. The large fullerenes C_{92} and C_{112} and the small fullerene C_{24} could be used to catalyze the oxidation of water to peroxide through their first metastable anions as well as serve as an inexpensive single nanocatalyst for water purification in the developing world [8].

Conundrum in measured electron affinities of heavy atoms: Recently, the EA of atomic Eu was measured to be 0.116 ± 0.013 eV [9]. This value is in outstanding agreement with the values of the Regge pole [10] and MCDF-RCI [11] methods. Previously, the EA of Eu was measured to be 1.053 $\pm$ 0.025 eV [12], which agrees excellently with the Regge pole value of 1.085 eV. Here we have a conundrum because an atom can have only a single EA. Also, a recent experiment [13] measured the EA of Nb and obtained generally good agreement with existing theoretical EAs, including ours which corresponds to the BE of an excited state. Our Nb^- ground state BE is 2.48 eV. The quandary requires that the measured EAs above, including those for Gd, Tb and Tm be reinterpreted.

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