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Negative ion formation in low-energy electron-fullerene collisions: Fullerene anionic catalysis[1] ZINEB FELFLI, KELVIN SUGGS, NANTAMBU NICHOLAS, ALFRED Z MSEZANE, Clark Atlanta Univ — Negative-ion formation in the fullerene molecules C_{44}, C_{60}, C_{100}, C_{124}, C_{128} and C_{136} is explored through low-energy electron elastic scattering total cross sections (TCSs) calculations using our robust Regge-pole methodology. We find that the TCSs are characterized generally by ground, metastable and excited negative ion formation during the collisions, Ramsauer-Townsend minima and shape resonances. The novelty and generality of the Regge-pole approach is in the extraction of the negative ion binding energies (BEs) of complex heavy systems from the calculated TCSs. For ground states collisions these BEs correspond to the electron affinities (EAs), yielding excellent agreement with measured EAs for C_{20} through C_{92} [1, 2]. Utility of the formed fullerene negative ions is demonstrated in the catalysis of water oxidation to peroxide and water synthesis from H_2 and O_2 using the anionic fullerene catalysts C_{20} - C_{136}. DFT transition state calculations found $C_{52}$and C_{60} numerically stable for both water and peroxide synthesis, C_{100} increases the energy barrier the most and C_{136} the most effective catalyst in both water synthesis and oxidation to H_2O_2.

1. A. Z. Msezane and Z. Felfli, Chem. Phys. **503**, 50 (2018)

2. Z. Felfli and A.Z. Msezane, Euro. Phys. J. D **72**, 78 (2018)

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