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Electron-impact total ionization cross sections of DNA sugar-phosphate backbone and an additivity principle WINIFRED HUO, NASA Ames Research Center, CHRISTOPHER DATEO, ELORET Corporation — The improved binary-encounter dipole (iBED) model [W.M. Huo, Phys. Rev. A64, 042719-1 (2001)] is used to study the total ionization cross sections of the DNA sugar-phosphate backbone by electron impact. Calculations using neutral fragments found that the total ionization cross sections of C3′- and C5′-deoxyribose- phospate, two conformers of the sugar-phosphate backbone, are close to each other. Furthermore, the sum of the ionization cross sections of the separate deoxyribose and phosphate fragments is in close agreement with the C3′- and C5′- deoxyribose-phospate cross sections, differing by less than 10%. The result implies that certain properties of the DNA, like the total singly ionization cross section, are localized properties and a building-up or additivity principle may apply. This allows us to obtain accurate properties of larger molecular systems built up from the results of smaller subsystem fragments. Calculations are underway using a negatively charged sugar- phosphate backbone with a metal counter-ion.

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