

The study of energy spectrum of the homonuclear quasi-molecules in the critical region

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In the present work critical distances for homonuclear quasi-molecules are calculated for a range of point-like and extended nuclei with $85 < Z < 100$. High-precision relativistic calculations of the ground-state energy of molecular ions with charges $Z = 1, 2, 10, 20, 30, 40, 50, 60, 70, 80, 90, 92, 100$ at “chemical distances” $R = 2/Z$ (in a.u.) were executed. To solve the two-centered Dirac equation the Dirac-Fock-Sturm method, based on the Dirac-Sturm orbitals application for constructing Dirac wave functions is used. According to this method wave functions represent a set of Dirac-Sturm basic functions, which are central-field 4-component Dirac bispinors centred at the ions. The radial parts of these orbitals are obtained by solving numerically the finite-difference radial one-center Dirac and Dirac-Sturm equations.

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