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Spectral characteristics of three-particle ionic molecular system of the exotic Carbon atom in one-dimensional space

The work presents results of calculations of the spectral characteristics for three-particle molecular ions of the Carbon atom

$$C^{6+}e^{\pm}\overline{C^{6+}}$$

Calculations for these systems had been carried out within the framework of the non-relativistic quantum-mechanical model for the three-body problem, which is based on relative collective Jacobian variables [1]. To find partial solutions of the non-relativistic Schrödinger equation (NRSh) from three independent variables, the problem is reduced to solving two boundary problems - finding adiabatic potentials - $U_v(R)$ and energy values (ε) of the ground and excited states of odd-even (oe) and even-even (ee) series of the given system. After separating the movement of the center of mass system, the NRSh depends only on two independent variables (R,α). The radial variable (R) belongs to the interval [0,∞), and the variable α is within the interval [0,β], where β is determined by the particle's mass [1]. Since the potential energy operator is singular, we will use the scalable multiplier (proposed by Hiroshi Nakatsuji [2]) to eliminate the singular points determined by the masses of the considered system. The introduction of a scalable multiplier is a procedure equivalent to the transition to a non-orthogonal basis, which leads to the generalized problem on eigenvalues and eigenfunctions.

The coordinates' values of the adiabatic potential energies minima for the considered series are respectively:

$$[-5.02076081003489*10^{16},[r=1.56250000000000*10^{(-8)}]]$$ - for even-even

$$[-1.2577263633462*10^{17},[r=1.22070312500000*10^{(-8)}]]$$ - for odd-even series

Numerical calculations of adiabatic potentials for series (ee) and (oe) and spectral parameters of the considered system were carried out using the Maple program (2017).

Results of these calculations are presented in the table.

States	Energy values of states ε (eV)	Average radius of the state, <r> (a.u.)	Average radius of the system, (m)
$^1S^{ee}_{Ce\bar{e}}\varepsilon_{00}$	$3.057105434\cdot10^{16}$	$2\cdot10^{-9}$	
$^1S^{ee}_{Ce\bar{e}}\varepsilon_{01}$	$5.469531600\cdot10^{12}$	$2\cdot10^{-8}$	$1.058\cdot10^{-18}$
$^1S^{oe}_{C\bar{C}}\varepsilon_{00}$	$6.382967840\cdot10^{15}$	$3.5\cdot10^{-9}$	
$^1S^{oe}_{C\bar{C}}\varepsilon_{01}$	$2.721160000\cdot10^{14}$	$125\cdot10^{-10}$	$6.6125\cdot10^{-19}$

The obtained energy values of the ground and excited states of the considered system lie in the range of ~[$3.06\cdot10^{16}$, $5.47\cdot10^{12}$] eV. It should be noted that the Hamiltonian of this system is invariant, since when the charge of each particle of a given ion is replaced by corresponding antiparticle, we received the same parameters for negative ions. Positive ions, attracting negative ions, will form neutral molecules of six-particle type [3].

The received data allow us to assume the existence of molecular Carbon ions, and the applied mathematical approach can be used in performing calculations for other systems

[1] M. I. Haysak, I. I. Haysak, M. Nagy, V. V. Onysko, Acta Physica Polonica A, 142 (4), 549 (2022). http://dx.doi.org/10.12693/APhysPolA.142.549.
[2] Nakatsuji H. Scaled Schrödinger Equation and the Exact Wave Function. Phys. Rev. Lett. 2004;93:030403. https://doi.org/10.1103/PhysRevLett.93.030403.
[3] J. Wolfe & A. Mysyrowicz, Excitonic Matter. Scientific American, 250(3), 98-107 (1984) Retrieved October 12, 2020, from http://www.jstor.org/stable/24969326.

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