NOTIZEN

Simple Analytical Eigenfunctions of Electrons in Thomas–Fermi Atoms

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Analytical solutions of the Schrödinger equation for the approximate Thomas–Fermi potential have been given by Kerner [1] and others [2]. The author [2] has obtained his functions using a more accurate approximate potential, but the obtained eigenfunctions are not simple for practical purposes. It is the purpose of this note to give analytical solutions for practical use of the Schrödinger equation for the approximate Thomas–Fermi potential of the author. The Schrödinger equation for the author's approximate potential in atomic units is

$$y_l'' + \left[-\alpha^2 + \frac{2Z}{r(1+Ar)^2} - \frac{l(l+1)}{r^2}\right] y_l = 0\,, \quad (1)$$

where Z = atomic number and $A = 0.64309\, Z^{1/3}$. The radial part $R_l(r) = y_l(r)/r$ may be written in the form

$$y_l(r) = e^{-\alpha r}\left(\frac{Ar}{1+Ar}\right)^{l+1} f(x)\,, \quad (2)$$

where $x = Ar/(1+Ar)$. Substituting $y_l(r)$ in the Schrödinger equation, we see that $f(x)$ fulfills the differential equation

$$x(x-1)^2 f'' + 2\left[l+1-\left(2l+3+\frac{\alpha}{A}\right)x + (l+2)\,x^2\right] f' + \left[\frac{2Z}{A} - 2(l+1)^2 - \frac{2\alpha}{A}(l+1) + (l+1)(l+2)\,x - \frac{2Z}{A}\,x\right] f = 0\,. \quad (3)$$

If we set $f(x) = \sum_{\nu=0}^{\infty} c_\nu x^\nu$ we obtain the following recurrence formulas for the c_ν:

$$\left[(\nu-1)(\nu+2l+2) + (l+1)(l+2) - \frac{2Z}{A}\right] c_{\nu-1} + 2\left[\frac{Z}{A} - (l+1)^2 - \frac{\alpha}{A}(l+\nu+1) - \nu(2l+\nu+2)\right] c_\nu + (\nu+1)(\nu+2l+2)\, c_{\nu+1} = 0 \quad (4)$$

valid for $\nu = 0, 1, 2, \ldots$ and $c_{-1} = 0$. Setting $A = 0$ we obtain the well known recurrence formulas for an electron in the field of a bare nucleus where $n = l+1+\nu$ is the principal quantum number. Rewriting the recurrence formulas given by Eq. (4) in the quantum numbers n, l we have

$$\left[n(n-1) - \frac{2Z}{A}\right] c_{n-l-2} + 2\left[\frac{A}{Z} - \frac{\alpha n}{A} - n^2\right] c_{n-l-1} + (n-l)(n+l+1)\, c_{n-l} = 0\,. \quad (5)$$

Neglecting the coefficient c_{n-l-1} in Eq. (5) gives us the zero approximation for the eigenvalue $\alpha_0 = Z/n - nA$. In order to obtain the first approximation of the eigenvalue α_1 we apply the same procedure which has been previously used by the author [3]. At first we write the following determinant

$$\begin{vmatrix} 2\left[\frac{Z}{A}\frac{\alpha}{A}(n-1) - (n-1)^2\right] & (n-l-1)(n+l) & 0 \\ n(n-1) - \frac{2Z}{A} & 2\left[\frac{Z}{A}\frac{\alpha n}{A} - n^2\right] & (n-l)(n+l+1) \\ 0 & n(n+1) - \frac{2Z}{A} & 2\left[\frac{Z}{A}\frac{\alpha}{A}(n+1) - (n+1)^2\right] \end{vmatrix} = 0 \quad (6)$$

which follows directly from the recurrence formulas given by Eq. (5). If we set $\alpha = \alpha_0$ in the corner terms of this determinant we then obtain the first order equation for α_1

$$\alpha_1 = \frac{Z}{n} - nA - \frac{(n-l)(n+l+1)[2Z - n(n+1)A]A}{4[Z+n(n+1)A]} + \frac{(n-l-1)(n+l)[2Z - n(n-1)A]A}{4[Z+n(n-1)A]}\,. \quad (7)$$

[1] E. H. Kerner, Phys. Rev. **83**, 71 [1951].
[2] T. Tietz, J. Chem. Phys. **25**, 787 [1956], and H. J. W. Müller, Ann. Phys. **16**, 255 [1965].
[3] For reference see ref. [2].

Table 1 gives a comparison of our results α_1 for the 1s-state with Latter's results [4] for several Z-values.

Z	8	10	13	19	26	29	37	47	57	65	74	82	92
(a)	6.092	—	10.536	16.022	22.546	25.365	32.939	42.485	51.971	59.800	68.498	76.250	85.965
(b)	5.897	7.680	10.260	15.962	22.455	25.404	33.048	42.672	52.347	59.785	68.348	76.722	85.769

Table 1. A comparison of our results (b) with Latter's results (a) for the 1s-state and several Z-values.

Table 2 shows a comparison of our approximate eigenvalues α_1 for $Z=80$ with the corresponding Hartree eigenvalues for several quantum numbers.

States	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
α_1 Eq. (7)	74.728	30.794	30.348	15.218	14.713	13.702	7.521	7.041	6.079	4.638
Hartree	74.48	30.41	29.87	14.76	14.19	13.08	6.87	6.34	5.27	3.09

Table 2. A comparison of our approximate eigenvalues α_1 given by Eq. (7) for $Z=80$ with the corresponding Hartree-values.

Table 1 and 2 show that the approximate eigenvalues calculated by help of Eq. (7) give reasonable results. In order to obtain more accurate eigenvalues than those given by α_1 we must solve a determinant of higher order than that in Eq. (6). The corresponding eigenfunctions for practical purpose are obtained from Eqs. (2) and (5) by respecting only finite numbers of the coefficients c_{n-l-1} so that the eigenfunctions show the proper numbers of zeroes. Eq. (2) shows that the eigenfunctions have accurate behavior for $r=0$ and $r \to \infty$.

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Reactivity Indices in Benzotropones

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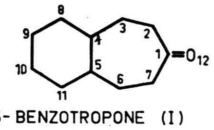
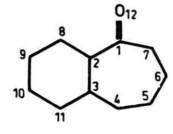
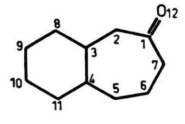
The present communication reports a theoretical study of the reactivity indices of tropones fused with a benzene ring; the so-called benzotropones. There are three possible benzotropones: 4,5-benzotropone, 2,3-benzotropone, and 3,4-benzotropone, shown in Fig. 1. Several research workers [1–9] have reported the syntheses and properties of 4,5-benzotropone and 2,3-benzotropone. To our knowledge there is so far no synthesis of 3,4-benzotropone reported in literature. We have investigated these molecules regarding substitution and addition reactions, being interested in predict-



4,5-BENZOTROPONE (I)



2,3-BENZOTROPONE (II)



3,4-BENZOTROPONE (III)

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