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Conclusions

Simple spectrophotometric method for the determination of NVP have been developed and validated according to ICH guidelines. The method is simple and easy to perform compared to other existing methods and do not entail any rigorous experimental variables which affect the reliability of the results. The ingredients usually present in the pharmaceutical formulations of these drugs seldom interfere in the proposed methods. The proposed method is simple, accurate and easy to perform and can be used for the routine determination of NVP in bulk and in dosage forms.

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Overview of Nikiforov-Uvarov (NU) Method

The NU method is based on the solutions of general second order linear differential equations with some orthogonal functions [7]. For the given potential, the Schrödinger equation in the spherical coordinates is reduced to a generalized equation of hyper-geometric type with an appropriate $s = s(r)$ coordinate transformation. Thus, it has the form [8]:

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \qquad (2)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. To find a particular solution of equation (2), we use the following transformation [9]:

$$\psi(s) = \phi(s)y(s) \qquad (3)$$

This reduces Schrödinger equation (2) to an equation of hyper-geometric type:

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0 \qquad (4)$$

where $\phi(s)$ satisfies $\phi'(s)/\phi(s) = \pi(s)/\sigma(s)$, y(s) is the hyper-geometric type function whose polynomial solutions are given by the Rodrigues relation:

$$y_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right] \qquad (5)$$

where B_n is a normalization constant and the weight function ρ must satisfy the condition [9]:

$$\left[\sigma(s)\rho(s)\right]' = \tau(s)\rho(s) \qquad (6)$$

The function π and the parameter λ required for this method are defined as:

$$\pi = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \qquad (7)$$

and

$$\lambda = k + \pi' \qquad (8)$$

Here, $\pi(s)$ is a polynomial with the parameter s and the determination of k is necessary for $\pi(s)$ to be obtained. To find k, the expression under the square root must be square of a polynomial. A new eigenvalue equation for the Schrödinger equation thus becomes:

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \quad (n = 0, 1, 2, \cdots), \qquad (9)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \qquad (10)$$

and $\tau'(s)$ must be negative.

Bound State Solutions via Nikiforov-Uvarov (NU) Method

The potential in equation (1) is substituted into the radial Schrödinger equation given as:

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r)\right]R_{n\ell}(r) = E_{n\ell}(r)R_{n\ell}(r), \qquad (11)$$

where n denotes the radial quantum number which together with ℓ are both named as the vibration-rotation quantum numbers in molecular chemistry, r is the internuclear separation, $E_{n\ell}$ is the exact bound state energy eigenvalues and V(r) is the internuclear potential energy function and we obtain:

$$\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{2}{r}\frac{dR_{n\ell}(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E_{n\ell} + \frac{a}{r} + \frac{a}{r}e^{-2br} + abe^{-2br} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R_{n\ell}(r) = 0. \qquad (12)$$

Equation (12) can be rearranged to give:

$$\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{2}{r}\frac{dR_{n\ell}(r)}{dr} + \frac{1}{r^2}\frac{2\mu}{\hbar^2}\left[\left(E_{n\ell} + abe^{-2br}\right)r^2 + \left(a + ae^{-2br}\right)r - \frac{\ell(\ell+1)\hbar^2}{2\mu}\right]R_{n\ell}(r) = 0. \qquad (13)$$

Introducing the following dimensional parameters:

$$\rho(r) = r^{1+\sqrt{4\gamma+1}} e^{-2i\varepsilon r}, \quad (31)$$

Substituting this into the Rodrigues relation given in equation (5), we get:

$$y_{n\ell}(r) = B_{n\ell} r^{-(1+\sqrt{4\gamma+1})} e^{2i\varepsilon r} \frac{d^n}{dr^n}\left[r^{(n+1+\sqrt{4\gamma+1})} e^{-2i\varepsilon r}\right] \quad (32)$$

$B_{n\ell}$ is the normalization constant. The polynomial solutions of $y_{n\ell}(r)$ in equation (32) are expressed in terms of the associated Laguerre polynomials, which is one of the orthogonal polynomials. We write:

$$y_{n\ell}(r) = L_n^{1+\sqrt{4\gamma+1}}(v), \quad (33)$$

where $v = 2i\varepsilon r$, therefore,

$$r = (2i\varepsilon)^{-1} v, \quad (34)$$

By substituting $\pi(r)$ and $\sigma(r)$ into the expression $\phi'(r)/\phi(r) = \pi(r)/\sigma(r)$ and solving the resulting differential equation, the other part of the wave function in equation (3) is obtained as:

$$\phi(r) = r^{\frac{1}{2}\sqrt{4\gamma+1}-\frac{1}{2}} e^{-i\varepsilon r} \quad (35)$$

or in terms of v,

$$\phi(v) = (2i\varepsilon)^{-\frac{3}{2}+\frac{1}{2}\sqrt{4\gamma+1}} v^{-\frac{1}{2}+\frac{1}{2}\sqrt{4\gamma+1}} e^{-\frac{v}{2}}, \quad (36)$$

Combining the Laguerre polynomials and $\phi(v)$ in equation (3), enables the radial wave function to be constructed as:

$$R_{n\ell}(r) = A_{n\ell}\psi_{n\ell}(r) \quad (37)$$

$$\therefore R_{n\ell}(r) = A_{n\ell}(2i\varepsilon)^{-\frac{3}{2}+\frac{1}{2}\sqrt{4\gamma+1}} v^{-\frac{1}{2}+\frac{1}{2}\sqrt{4\gamma+1}} e^{-\frac{v}{2}} L_n^{1+\sqrt{4\gamma+1}}(v), \quad (38)$$

If we introduce the variable $\alpha = \frac{1}{2}\sqrt{4\gamma+1}$, equation (38) becomes:

$$R_{n\ell}(r) = A_{n\ell}(2i\varepsilon)^{-\frac{3}{2}+\alpha} v^{-\frac{1}{2}+\alpha} e^{-\frac{v}{2}} L_n^{1+2\alpha}(v), \quad (39)$$

To find $A_{n\ell}$, a new normalization constant, we write:

$$\int_0^\infty R_{n\ell}^2(r)\,dr = 1. \quad (40)$$

Therefore,

$$A_{n\ell}^2 (2i\varepsilon)^{2\alpha-3} \int_0^\infty v^{2\alpha-1} e^{-v}\left[L_n^{2\alpha+1}(v)\right]^2 dv = 1. \quad (41)$$

The above integral can be evaluated by using the recursion relation for Laguerre polynomials and $A_{n\ell}$ is found to be:

$$A_{n\ell} = \left[\frac{(n-2\alpha+1)!(2i\varepsilon)^{3-2\alpha}}{(2n-2\alpha+2)(n!)^3}\right]^{\frac{1}{2}} \quad (42)$$

Therefore, $R_{n\ell}(r)$ becomes:

$$R_{n\ell}(r) = \left[\frac{(n-2\alpha+1)!(2i\varepsilon)^{3-2\alpha}}{(2n-2\alpha+2)(n!)^3}\right]^{\frac{1}{2}} (2i\varepsilon)^{-\frac{3}{2}+\alpha} v^{\alpha-\frac{1}{2}} e^{-\frac{v}{2}} L_n^{2\alpha+1}(v). \quad (43)$$

Conclusion

The analytical solutions of the Schrödinger equation for the general exponential screened coulomb potential has been presented. The Nikiforov-Uvarov method employed in the solutions enables us to explore an effective way of obtaining the eigenvalues and corresponding eigenfunctions of the Schrödinger equation for any ℓ - state.

Finally, we calculate the energies of the exponential screened coulomb potential for diatomic molecules by means of equation (30) for the ℓ - state. The explicit values of the energy at different values of the screened parameter are shown in Table 1.

Table 1. Bound State Eigenvalues for $0 \le b \le 0.5$ for the 1s State of Diatomic Molecules in Atomic Units $(\hbar = \mu = a = 1)$