Use of Coulomb-Yukawa Like Correlated Interaction Potentials of Integer and Noninteger Indices and One-range Addition Theorems for ψ^α-ETO in Evaluation of Potential of Electric Field Produced by Molecule

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Using Coulomb-Yukawa like correlated interaction potentials of integer and noninteger indices the series expansion formulae in terms of multicenter overlap integrals of three complete orthonormal sets of ψ^α-exponential type orbitals and linear combination coefficients of molecular orbitals are established for the potential of electrostatic field produced by the charges of molecule, where $\alpha = 1, 0, -1, -2, \cdots$. The formulae obtained can be useful for the study of interaction between atomic-molecular systems containing any number of closed and open shells when the ψ^α-exponential type basis functions and Coulomb-Yukawa like correlated interaction potentials are used in the Hartree-Fock-Roothaan and explicitly correlated approximations. The final results are valid for the arbitrary values of parameters of correlated interaction potentials and orbitals. As an example of application, the calculations have been performed for the potential energy of interaction between electron and molecule H_2O using combined Hartree-Fock-Roothaan equations suggested by the author.

Key Words: ψ^α-exponential type orbitals, Coulomb-Yukawa like interaction potentials. Addition theorems, Hartree-Fock-Roothaan approximation

Introduction

It is well known that the electron-molecule interaction potential is very sensitive to the minor errors in the wave functions.[1,2] Therefore, for the caculation of this potential it is desirable to use Slater type orbitals (STO) as basis sets which describe the situation more accurately than do Gaussion type orbitals. In the study of electron-molecule interaction the Slater functions were used in the literature (see Refs. [3-6] and the bibliography quoted in these papers).Unfortunately, the STO functions are not orthogonal with respect to the principal quantum numbers that creates some difficulties in electron-molecule potential calculations. Thus, the neccessity for using the complete orthonormal sets of ψ^α-exponential type orbitals ($\psi^\alpha - ETO$, $\alpha = 1, 0, -1, -2, \cdots$) as basis functions arises.[7] In previous papers,[8,9] a large number of different sets of expansion formulae of symmetrical and unsymmetrical one-range addition theorems and multicenter charge densities for $\psi^\alpha - ETO$ basis funtions has been established. These different sets have the further advantages that the formulae presented in Refs. [8,9] can be chosen properly according to the nature of the problems under consideration. This is rather important because the choice of series expansion relations will determine the rate of convergence of series expansions arising in molecular electronic structure calculations.

In this study, the series of expansion formulae are derived for the potential produced by molecule when the $\psi^\alpha - ETO$ basis functions and the Coulomb-Yukawa like correlated interaction potentials (CIP) approximations in the Hartree-Fock-Roothaan (HFR) theory are employed. The results presented are especially useful for the investigation of electron scattaring from molecules and interaction between them.

Definition and Basic Formulas

The operator of noninteger μ^- potential examined in this work has the following form (see Fig. 1):

$$\hat{\varphi}^{\mu^- v\sigma}(\xi, \vec{r}_{og}) = \sum_b Z_b \hat{h}^{\mu^- v\sigma}(\xi, \vec{r}_{bg}) - \sum_{i=1}^N \hat{h}^{\mu^- v\sigma}(\xi, \vec{r}_{ig}). \quad (1)$$

Here, $\vec{r}_{og}$ and $\vec{r}_{bg}$ are radius-vectors of the point g with respect to the origin of the molecular coordinate system and to the nuclei of N electron molecule, respectively ($b \equiv a, c, \ldots$). Z_b is the charge of nucleus b. r_{ig} is the distance to the ith electron of molecule and $0 \leq \xi < \infty$. The Coulomb (*for* $\xi = 0$) and Yukawa (*for* $\xi \neq 0$) like CIP operators occurring in Eq.(1) are defined as[10]

$$\hat{h}^{\mu^- v\sigma}(\xi, \vec{r}) = \left(\frac{4\pi}{2v+1}\right)^{\frac{1}{2}} r^{\mu^-l} e^{-\xi r} S_{v\sigma}(\theta, \varphi), \quad (2)$$

where $S_{v\sigma}(\theta, \varphi)$ are the complex ($S_{v\sigma} \equiv Y_{v\sigma}$) or real spherical hormonics.

In order to obtain the average expectation value of operator (1) we shall use the complete sets of $\psi^\alpha - ETO$ and $\bar{\psi}^\alpha - ETO$ basis functions defined by[7]

$$\Psi_{nlm}^\alpha(\zeta, \vec{r}) = R_{nl}^\alpha(\zeta, r) S_{lm}(\theta, \varphi) \quad (3)$$

$$\bar{\Psi}_{nlm}^\alpha(\zeta, \vec{r}) = \left(\frac{2n}{x}\right)^\alpha \Psi_{nlm}^\alpha(\zeta, \vec{r}) \quad (4)$$

$$R_{nl}^\alpha(\zeta, r) = (-1)^\alpha \left[\frac{(2\zeta)^3 (q-p)!}{(2n)^\alpha (q!)^3}\right]^{1/2} x^l e^{-x/2} L_q^p(x), \quad (5)$$

where $a = 1, 0, -1, -2, \ldots, p = 2l + 2 - a, q = n + l + 1 - a, x = 2\zeta r$ and $L_q^p(x)$ is the generalized Laguerre polynomial. The $\psi^a - ETO$ and $\overline{\psi}^a - ETO$ satisfy the following orthonormality relation:

$$\int \Psi_{nlm}^{a*}(\zeta, \vec{r}) \, \overline{\Psi}_{n'l'm'}^{a}(\zeta, \vec{r}) dv = \delta_{nn'}\delta_{ll'}\delta_{mm'}. \tag{6}$$

One-center Expansion Formulae for Potential Operator in Terms of $\psi^a - ETO$

In the treatment of potential of the field produced by all the charges of molecule it is necessary to transform the operator (1), which depends upon the coordinates of three points, in such a way that the coordinates of these points appear in a computationally more convenient form. This requires a separation of integration variables from those related to the geometry of the molecule. For this purpose, we use the symmetrical one-range addition theorems established in a previous paper.[11] Then, using the $\psi^a - ETO$ and $\overline{\psi}^a - ETO$ basis functions determined by Eqs. (3) and (4) we obtain for one-center expansion of Cuolomb-Yukawa like noninteger μ^* CIP the expression in terms of integer μ CIP :

$$\hat{h}^{\mu'\nu\sigma}(\xi, \vec{r}) = \lim_{M \to \infty} \sum_{\mu=\nu+1}^{M} Q_{\mu'\nu,\mu\nu}^{aM}(\xi, \eta) h^{\mu\nu\sigma}(\eta, \vec{r}), \tag{7}$$

where $\eta > 0$ and

$$Q_{\mu'\nu,\mu\nu}^{aM}(\xi, \eta) = \sum_{\mu'=\nu-1}^{M} \Omega_{\mu\mu'}^{a\nu}(M) \frac{\Gamma(\mu^* + \mu' - a + 1)}{\left[\Gamma(2\mu+1)\Gamma(2\mu'-2a+1)\right]^{1/2}}$$
$$\times \frac{(2\eta)^{\mu'+\mu'-a-1}}{(\xi+\eta)^{\mu'+\mu'-a+1}} \tag{8}$$

$$\hat{h}^{\mu\nu\sigma}(\eta, \vec{r}) = \left(\frac{4\pi}{2\nu+1}\right)^{1/2} \frac{\sqrt{(2\mu)!}}{(2\eta)^{\mu+1/2}} \sum_{\mu'=\nu+1}^{\mu} \overline{\omega}_{\mu\mu'}^{a\nu} \Psi_{\mu'\nu\sigma}^{a}(\eta, \vec{r}). \tag{9}$$

Here,

$$\Omega_{\mu\mu'}^{a\nu}(M) = \left[\frac{[2(\mu'-a)]!}{(2\mu')!}\right]^{\frac{1}{2}} \sum_{\mu''=\max(\mu,\mu')}^{M} (2\mu'')^a \omega_{\mu''\mu}^{a\nu} \omega_{\mu''\mu'}^{a\nu} \tag{10}$$

$$\omega_{\mu\mu'}^{a\nu} = (-1)^{\mu'-\nu-1} \left[\frac{(\mu'+\nu+1)!}{(2\mu')^a(\mu'+\nu+1-a)!}\right.$$
$$\left. \times F_{\mu'+\nu+1-a}(\mu+\nu+1-a)F_{\mu'-\nu-1}(\mu-\nu-1)F_{\mu'-\nu-1}(2\mu')\right]^{1/2} \tag{11}$$

$$\overline{\omega}_{\mu\mu'}^{a\nu} = (-1)^{\mu'-\nu-1} \times$$
$$\left[\frac{(2\mu')^a(\mu+\nu+1-a)!F_{\mu'+\nu-1-a}(\mu+\nu+1-a)F_{\mu'-\nu-1}(\mu-\nu-1)}{(\mu+\nu+1)!F_{\mu'-\nu-1}(2\mu)}\right]^{1/2} \tag{12}$$

$$F_m(n) = \frac{n!}{m!(m-n)!}. \tag{13}$$

Substituting (9) into (7) we obtain for one-center expansion of Cuolomb-Yukawa like CIP operator in terms of $\psi^a - ETO$ the following formula:

$$\hat{h}^{\mu'\nu\sigma}(\xi, \vec{r}) = \sqrt{4\pi} \lim_{M \to \infty} \sum_{\mu=\nu+1}^{M} E_{\mu'\nu,\mu\nu}^{aM}(\xi, \eta) \Psi_{\mu\nu\sigma}^{a}(\eta, \vec{r}), \tag{14}$$

where

$$E_{\mu'\nu,\mu\nu}^{aM}(\xi, \eta) = \frac{1}{(2\nu+1)^{1/2}} \sum_{\mu'=\nu-1}^{M} \frac{\sqrt{(2\mu')!}}{(2\eta)^{\mu'+1/2}} \overline{\omega}_{\mu'\mu}^{a\nu} Q_{\mu'\nu,\mu\nu}^{aM}(\xi, \eta). \tag{15}$$

Use of Symmetrical One-range Addition Theorems of $\psi^a - ETO$

We take into account Eq. (14) in (1). Then, the potential operator is expressed through the basis functions $\psi^a - ETO$:

$$\hat{\phi}^{\mu'\nu\sigma}(\xi, \vec{r}_{og}) = \lim_{M \to \infty} \sum_{\mu=\nu-1}^{M} E_{\mu'\nu,\mu\nu}^{aM}(\xi, \eta) \hat{\phi}^{\mu\nu\sigma}(\eta, \vec{r}_{og}), \tag{16}$$

where

$$\hat{\phi}^{\mu\nu\sigma}(\eta, \vec{r}_{og}) = \sqrt{4\pi} \left\{\sum_b Z_b \Psi_{\mu\nu\sigma}^{a}(\eta, \vec{r}_{bg}) - \sum_{i=1}^{N} \Psi_{\mu\nu\sigma}^{a}(\eta, \vec{r}_{ig})\right\}. \tag{17}$$

Now we shall use in (17) the symmetrical one-range addition theorems of $\psi^a - ETO$ established in a previous paper[8] in the following form:

$$\Psi_{\mu\nu\sigma}^{a}(\eta, \vec{r}_{ig}) = \sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} V_{\mu\nu\sigma,nlm}^{-a}(\eta, \vec{r}_{og}) \overline{\Psi}_{nlm}^{a}(\eta, \vec{r}_{oi}), \tag{18}$$

where

$$V_{\mu\nu\sigma,nlm}^{-a}(\eta, \vec{r}_{og}) = (-1)^{\nu} \frac{\sqrt{4\pi}}{(2\eta)^{3/2}} \sum_{u=1}^{\infty}\sum_{v=0}^{u-1}\sum_{s=-v}^{v} d_{\mu\nu\sigma,nlm}^{a\,uvs} \Psi_{uvs}^{a*}(\eta, \vec{r}_{og}). \tag{19}$$

In the derivation of Eq. (19) we have taken into account the property $\Psi_{\mu\nu\sigma}^{a}(\eta, \vec{r}_{go}) = (-1)^{\nu} \Psi_{\mu\nu\sigma}^{a}(\eta, \vec{r}_{og})$ which is obtained by the use of inversion transformation of spherical harmonics. We notice that the quantities $V_{\mu\nu\sigma,nlm}^{-a}(\eta, \vec{r}_{og})$ are related to the radius vector of point where the potential of electric field produced by molecule is finding. Taking into account Eq. (18) in (17) we get for the separated form of potential operator $\hat{\phi}^{\mu\nu\sigma}$ the relation:

$$\hat{\phi}^{\mu\nu\sigma}(\eta, \vec{r}_{og}) = \sqrt{4\pi} \sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} V_{\mu\nu\sigma,nlm}^{-a}(\eta, \vec{r}_{og})$$
$$\times \left\{\sum_b Z_b \overline{\Psi}_{nlm}^{a}(\eta, \vec{R}_{ob}) - \sum_{i=1}^{N} \overline{\Psi}_{nlm}^{a}(\eta, \vec{r}_{oi})\right\}. \tag{20}$$

Using the method set out in Ref. [12] it is easy to show that the average expectation value of potential defined by Eq. (20) for multideterminantal single electron configuration states with any number of closed and open shells of molecule is given by the formula

$$\phi^{\mu\nu\sigma}(\eta,\vec{r}_{og}) = \sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} V^{\alpha}_{\mu\nu\sigma,nlm}(\eta,\vec{r}_{og})$$

$$\times \left\{\sqrt{4\pi}\sum_b Z_b \overline{\Psi}^{\alpha}_{nlm}(\eta,\vec{R}_{ob}) - 2\sum_i^{\kappa} f_i I^{\alpha}_{nlm,i}(\eta)\right\}, \quad (21)$$

where $\kappa = \kappa_c + \kappa_0$ is the number of occupied orbitals belonging to closed (κ_c) and open (κ_0) shells, f_i is the fractional occupancy of shell i and

$$I^{\alpha}_{nlm,i}(\eta) = \sqrt{4\pi}\int \Psi^{\alpha}_{nlm}(\eta,\vec{r}_{o1})u^{\alpha *}_i(\vec{r}_1)u^{\alpha}_i(\vec{r}_1)dv_1. \quad (22)$$

Here, are the molecular orbitals defined from the following linear combination of $\psi^{\alpha} - ETO$:

$$u^{\alpha}_i = \sum_p \Psi^{\alpha}_p C^{\alpha}_{pi}, \quad (23)$$

where $p \equiv nlm$. The linear combination coefficients C^{α}_{pi} can be determined by solving the combined HFR equations for molecule using $\psi^{\alpha} - ETO$ basis functions (see Ref. [12]). For the calculation of multicenter integrals arising in the combined HFR equations we can use the one-range addition theorems for basis functions (see Ref. [13] and references quoted therein to our papers).

The correlated interaction potential (21) can also be expanded in multipole potentials:

$$\phi^{\mu\nu\sigma}(\eta,\vec{r}_{og}) = \sum_{L=0}^{\infty}\sum_{M=-L}^{L} \phi^{\alpha\mu\nu\sigma}_{LM}(\eta,r_{og})S^*_{LM}(\theta_{og},\varphi_{og}), \quad (24)$$

where

$$\phi^{\alpha\mu\nu\sigma}_{LM}(\eta,r_{og}) = \int \phi^{\mu\nu\sigma}(\eta,\vec{r}_{og})S_{LM}(\theta_{og},\varphi_{og})d\Omega_{og}. \quad (25)$$

The evaluation of integral (25) can be performed using a formula (19). Then, it is easy to show that the radial part of multipole potential is determined by

$$\phi^{\alpha\mu\nu\sigma}_{LM}(\eta,r_{og}) = \sum_{N=L+1}^{\infty} \Pi^{\alpha NLM}_{\mu\nu\sigma}(\eta)R^{\alpha}_{NL}(\eta,r_{og}), \quad (26)$$

where $R^{\alpha}_{NL}(\eta,r_{og})$ is the radial part of $\psi^{\alpha} - ETO$ and

$$\Pi^{\alpha NLM}_{\mu\nu\sigma}(\eta) = (-1)^{l}\frac{\sqrt{4\pi}}{(2\eta)^{3/2}}\sum_{l=0}^{\infty}\sum_{-l}^{l}\sum_{-l}^{\infty} d^{\alpha NLM}_{\mu\nu\sigma,nlm}$$

$$\times \left\{\sqrt{4\pi}\sum_b Z_b \overline{\Psi}^{\alpha}_{nlm}(\eta,\vec{R}_{ob}) - 2\sum_i^{\kappa} f_i I^{\alpha}_{nlm,i}(\eta)\right\}. \quad (27)$$

Now we use in Eq. (22) the expression (23) for the molecular orbitals:

$$I^{\alpha}_{nlm,i}(\eta) \equiv I^{\alpha\,oo\kappa}_{nlm,i}(\eta) = \sum_{p_1}\sum_{p_1'} C^{\alpha *}_{p_1 i}C^{\alpha}_{p_1' i}S^{\alpha\,oo\kappa}_{p\,p_1\,p_1'}(\eta,\zeta_1,\zeta_1'), \quad (28)$$

where $p \equiv n_1 l_1 m_1$, $p_1' \equiv n_1' l_1' m_1'$ and $S^{\alpha\,oo\kappa}$ is the three-center overlap integral defined by

$$S^{\alpha oo\kappa}_{p\,p_1\,p_1'}(\eta,\zeta_1,\zeta_1') = \sqrt{4\pi}\int \overline{\Psi}^{\alpha}_p(\eta,\vec{r}_{o1})\Psi^{\alpha *}_{p_1}(\zeta_1,\vec{r}_{o1})\Psi^{\alpha}_{p_1'}(\zeta_1',\vec{r}_{c1})dv_1. \quad (29)$$

The series expansion relations for three-center integrals (29) in terms of two-center overlap integrals over $\psi^{\alpha} - ETO$ are presented in a previous work.[14]

Thus, we have established a large number of different sets of series expansion relations ($\alpha = 1, 0, -1, -2, \cdots$) for the potential produced by molecule in terms of linear combination coefficients of molecular orbitals and two-center overlap integrals over $\psi^{\alpha} - ETO$. For the calculation of two-center overlap integrals the efficient computer programs especially useful for large quantum numbers are available in our group.[15] Therefore, by using the computer programs for the overlap integrals one can calculate the potential of the field produced by molecule.

As an application of Eqs. (24) and (26) in the case of Coulomb interaction potential (for $u = v = \sigma = \xi = 0$), we have solved combined HFR equations[12] for the ground state of H_2O using the four different closed complete orthonormal sets of $\psi^{\alpha} - ETO$ as independent minimal basis functions, where $\alpha = 1, 0, -1, -2$. For this purpose, we have used for the atoms of H_2O the following coordinates (a. u.):

$$H(0, 1.4362, 1.1020), O(0, 0, 0), H(0, -1.4362, 1.1020).$$

The results of computer calculations in atomic units for $I^{\prime\alpha\,000}_{LM}(r_{og}) = -\phi^{\alpha\,000}_{LM}(r_{og})$ and $\phi^{\alpha\,000}(r_{og})$, where $\alpha = 1, 0, -1, -2$, are presented in Table 1 and Figure 2, respectively. As can be seen from Figure 2 that the molecule H_2O and its dipole moment lie on yz-plane, and the interaction potential is calculated on xz-plane. This potential is highest at around 35 degrees tilted as would be expected from classical electrostatics. Unfortunately, there are no previous results found in the literature to compare. Thus, in this work we have demonstrated the applicability of the one-range addition theorems of complete orthonormal sets of $\psi^{\alpha} - ETO$ to the study of potential of electric field produced by molecule.
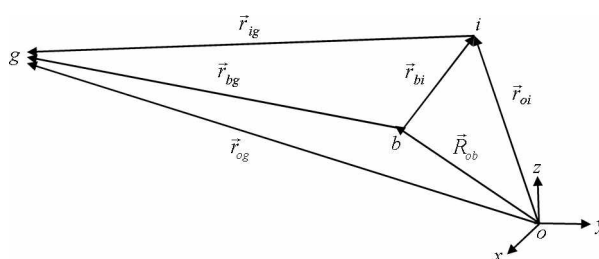

Figure 1. The position of charges of molecule and point g.

Table 1. The values of radial part of $I_{LM}^{\alpha\,000}$ for the potential energy of interaction between electron and H_2O for $\alpha = 1, 0, -1, -2$.

L	M	r_{og}														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	0	17.577	10.174	7.107	5.361	4.292	3.577	3.066	2.683	2.385	2.146	1.951	1.788	1.651	1.533	1.431
	1	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-0.800	-0.727	-0.667	-0.615	-0.571	-0.533
1	0	-8.452	-4.682	-2.877	-2.107	-1.668	-1.380	-1.177	-1.026	-0.810	-0.817	-0.741	-0.678	-0.625	-0.580	-0.541
	-1	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-0.800	-0.727	-0.667	-0.615	-0.571	-0.533
	2	-8.098	-4.501	-2.781	-2.046	-1.624	-1.347	-1.151	-1.006	-0.893	-0.803	-0.729	-0.668	-0.617	-0.572	-0.534
	1	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.899	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
2	0	-8.142	-4.143	-2.717	-2.022	-1.611	-1.340	-1.147	-1.003	-0.891	-8.001	-0.728	-0.675	-0.616	-0.572	-0.534
	-1	-8.000	-4.000	-2.677	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
	-2	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
	3	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
	2	-8.074	-4.612	-2.752	-2.022	-1.609	-1.338	-1.145	-1.000	-0.890	-8.000	-0.728	-0.667	-0.616	-0.572	-0.534
	1	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.001	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
3	0	-7.946	-3.697	-2.621	-1.987	-1.595	-1.331	-1.142	-1.000	-0.888	-0.799	-0.727	-0.666	-0.615	-0.571	-0.533
	-1	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-0.999	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
	-2	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
	-3	-8.000	-4.000	-2.667	-2.000	-1.600	-1.333	-1.143	-1.000	-0.889	-8.000	-0.727	-0.667	-0.615	-0.571	-0.533
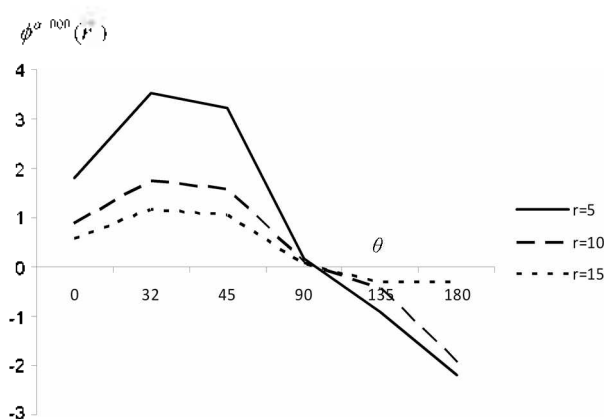
Figure 2. Dependence of the potential $\phi^{\alpha\,000}(r_{og})$ produced by H_2O on θ_{og} for $\varphi_{og} = 0$, $r_{og} = 5, 10, 15$ and $\alpha = 1, 0, -1, -2$.

Conclusion

The reliable descriptions of interaction between molecules, electron scattering from molecules and their photoionization and photoluminescence require *ab initio* electron-molecule potential. In this study, the computationally efficient and accurate method for evaluating electron-molecule interaction potentials has been suggested using one-range addition theorems for $\psi^{\alpha} - ETO$.[8,9] The series expansion formulae are expressed through the linear combination coefficients of molecular orbitals and multicenter overlap integrals of $\psi^{\alpha} - ETO$. The electron-molecule interaction potentials obtained are of great importance from the viewpoint of both theory as well as their application especially to the determination of interaction energy between atomic-molecular systems when the HFR and explicitly correlated approaches are employed.

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