

Research Article

Evaluation of Self-Friction Three-Center Nuclear Attraction Integrals with Integer and Noninteger Principal Quantum Numbers n over Slater Type Orbitals

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Received 2 November 2016; Revised 7 February 2017; Accepted 21 February 2017; Published 6 March 2017

Academic Editor: Demeter Tzeli

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We have proposed a new approach to evaluate self-friction (SF) three-center nuclear attraction integrals over integer and noninteger Slater type orbitals (STOs) by using Guseinov one-range addition theorem in standard convention. A complete orthonormal set of Guseinov $\psi^{(\alpha)}$ exponential type orbitals ($\psi^{(\alpha)}$ -ETOs, $\alpha = 2, 1, 0, -1, -2, \dots$) has been used to obtain the analytical expressions. The overlap integrals with noninteger quantum numbers occurring in SF three-center nuclear attraction integrals have been evaluated using Q_{ns}^q auxiliary functions. The accuracy of obtained formulas is satisfactory for arbitrary integer and noninteger principal quantum numbers.

1. Introduction

It is well known that Roothaan open-shell Hartree-Fock theory (HFR) and its extensions are not, in general, applicable to any state of a single configuration, which has any symmetry of open shells [1–10]. In a recent paper [11], Guseinov has eliminated the insufficiencies arising in HFR theory and has suggested a combined open-shell Hartree-Fock-Roothaan theory (CHFR) which includes the arbitrary number and symmetry of closed- and open-shell cases. It is clear that the evaluation of multicenter molecular integrals arising in CHFR theory has prime importance in many branches of physics particularly quantum physics, atomic and molecular physics, and nuclear physics. Using different approximations, considerable efforts have been made for calculating these integrals over STOs with noninteger principal quantum numbers n (NISTOs). Notice that the NISTOs describe the physical systems more accurately than do ISTOs with integer principal quantum numbers [12–17]. But the main problem of using NISTOs basis in molecular calculations arises in the evaluation of the multicenter integrals. Various methods have been proposed in the literature for improving evaluation for the use of NISTOs in molecular calculations. It should be noted that most of the studies in the literature on the

evaluation of multicenter molecular integrals with NISTOs were not entirely successful [18–20].

According to classical electrodynamics, the Lagrangian for a system of charges does not include the Lorentz self-friction (SF) potentials [21–23]. By considering this deficiency, Guseinov had suggested a new centrally symmetric potential of the SF field and on the basis of this idea Guseinov proposed the new complete orthonormal sets of $\psi^{(\alpha)}$ -ETOs. The indices α arising from the use of total potential and occurring in the Guseinov $\psi^{(\alpha)}$ -ETOs are the frictional quantum number. For the evaluation of multicenter molecular integrals of integer Slater type orbitals (ISTOs) and noninteger Slater type orbitals (NISTOs) appearing in the CHFR approximation, Guseinov derived one-range addition theorems by the use of complete orthonormal sets of Guseinov $\psi^{(\alpha)}$ -ETOs [24].

In this case the analytical formulas for the evaluation of multicenter molecular integrals are directly depending on the SF quantum number. Thus, considering SF interactions, the calculation results of physical and chemical properties of atoms and molecules obtained from CHFR equations are closer to their real values. Therefore, the new type of multicenter molecular integrals arising in CHFR equations should be called SF multicenter molecular integrals. SF

three-center nuclear attraction integral is one of the most important molecular integrals arising in CHFR equations.

The aim of this paper is to provide the general analytical expressions of SF three-center nuclear attraction integrals over ISTOs and NISTOs. With the help of Guseinov one-range addition theorems and $\psi^{(\alpha)}$ -ETOs, we have established new algorithm for calculating SF three-center nuclear attraction integrals. We noticed that the SF three-center nuclear attraction integrals are expressed in terms of two-center overlap integrals and two-center nuclear attraction integrals over NISTOs. The convergence, accuracy, and CPU time have been tested by our previous studies.

2. Definitions and Basic Formulas

The ISTOs can be written as follows [25, 26]:

$$\chi_{nlm}(\zeta, \vec{r}) = (2\zeta)^{n+1/2} [(2n)!]^{-1/2} r^{n-1} e^{-\zeta r} S_{lm}(\theta, \varphi), \quad (1)$$

$$\chi_{n^*lm}(\zeta, \vec{r}_a) = \sum_{\nu=0}^{N-1} \sum_{\sigma=-\nu}^{\nu} \sum_{i=\nu+1}^N \sum_{j=\nu+1}^i \left[\frac{[2(j-\alpha)!]}{(2j)!} \right]^{1/2} (2i)^\alpha \omega_{ij}^{\alpha\gamma} S_{n^*lm, j-\alpha\nu\sigma}(\zeta, \zeta; \vec{R}) \sum_{\mu=\nu+1}^i \omega_{i\mu}^{\alpha\gamma} \chi_{\mu\nu\sigma}(\zeta, \vec{r}_b), \quad (3)$$

where $\vec{R} \equiv \vec{R}_{ab}$, $\alpha = 2, 1, 0, -1, -2, \dots$, and the coefficients $\omega_{\mu\mu'}^{\alpha\gamma}$ are determined as follows:

$$\begin{aligned} \omega_{\mu\mu'}^{\alpha\gamma} &= (-1)^{\mu'-\nu-1} \left[\frac{(\mu' + \nu + 1)!}{(2\mu)^\alpha (\mu' + \nu + 1 - \alpha)!} \right. \\ &\cdot F_{\mu'+\nu+1-\alpha}(\mu + \nu + 1 - \alpha) F_{\mu'-\nu-1}(\mu - \nu - 1) \quad (4) \\ &\left. \cdot F_{\mu'-\nu-1}(2\mu') \right]^{1/2}. \end{aligned}$$

In (3) and (4), $F_\mu(k) = k!/\lfloor \mu!(k-\mu)! \rfloor$ and the quantities $S_{n^*lm, \mu\nu\sigma}$ are the overlap integrals between the NISTOs and ISTOs:

$$S_{n^*lm, \mu\nu\sigma}(\zeta, \zeta; \vec{R}) = \int \chi_{n^*lm}^*(\zeta, \vec{r}_a) \chi_{\mu\nu\sigma}(\zeta, \vec{r}_b) dV. \quad (5)$$

For the evaluation of $S_{n^*lm, \mu\nu\sigma}$ overlap integrals we use the formula defined in terms of Q_{ns}^q auxiliary functions [30]. As

where n is an integer principal quantum number, ζ is the screening constant, and $S_{lm}(\theta, \varphi)$ is a complex or real spherical harmonic (see [27–29] for exact definitions).

The NISTOs with noninteger values of the principal quantum number n^* are defined by

$$\begin{aligned} \chi_{n^*lm}(\zeta, \vec{r}) \\ = (2\zeta)^{n^*+1/2} [\Gamma(2n^* + 1)]^{-1/2} r^{n^*-1} e^{-\zeta r} S_{lm}(\theta, \varphi). \end{aligned} \quad (2)$$

Here, $\Gamma(x)$ is the gamma function.

To obtain the expansion of NISTOs about a new center by the use of complete orthonormal sets of Ψ^α -ETOs we can use the method for the expansion of ISTOs. Finally the formulas for the expansion of NISTOs in terms of ISTOs at a new origin are defined as [24]

can be seen from (3), the coefficients for expansion of NISTOs for $R \neq 0$ are expressed through the noninteger n^* overlap integrals with the same screening constants defined by (5). It is clear that the obtained expansion formulas from this paper can also be used in the case of integer values of n^* . Equation (3) becomes the series expansion formulas for translation of ISTOs (see, (5) of [31]).

3. Evaluation of SF Three-Center Nuclear Attraction Integrals

The SF three-center nuclear attraction integrals over NISTOs are defined by

$$\begin{aligned} I_{n^*lm, n'^* l'm'}(\zeta, \zeta', \vec{R}_{ca}, \vec{R}_{ab}) \\ = \int \chi_{n^*lm}^*(\zeta, \vec{r}_a) \chi_{n'^*l'm'}(\zeta', \vec{r}_c) \frac{1}{r_b} dV, \end{aligned} \quad (6)$$

where $\vec{R}_{ab} = \vec{r}_a - \vec{r}_b$ and $\vec{R}_{ca} = \vec{r}_c - \vec{r}_a$.

Taking into account (3) in (6) we obtain the following relations:

$$\begin{aligned} I_{n^*lm, n'^* l'm'}^\alpha(\zeta, \zeta', \vec{R}_{ca}, \vec{R}_{ab}) \\ = \sum_{\nu=0}^{N-1} \sum_{\sigma=-\nu}^{\nu} \sum_{i=\nu+1}^N \sum_{j=\nu+1}^i \omega_{ij}^{\alpha\gamma} S_{n'^*l'm', j-\alpha\nu\sigma}(\zeta', \zeta', R_{ac}) \left[\frac{[2(j-\alpha)!]}{(2j)!} \right]^{1/2} (2i)^\alpha \sum_{\mu=\nu+1}^i \omega_{i\mu}^{\alpha\gamma} I_{n^*lm, \mu\nu\sigma}(\zeta, \zeta', R_{ab}). \end{aligned} \quad (7)$$

TABLE 1: Comparison methods of computing integer and noninteger SF three-center nuclear attraction integrals over STOs obtained in the molecular coordinate system for $N = 15$ (in a.u.).

n^*	l	m	ζ	n'^*	l'	m'	ζ'	R_{ca}	θ_{ca}	ϕ_{ca}	R_{ab}	θ_{ab}	ϕ_{ab}	Eq. (7)	
														$\alpha = 0$	$\alpha = 1$
1.1	0	0	7.6	1.1	0	0	3.4	2.1	108	300	1.4	60	180	2.5334592872E - 3	2.5349685569E - 3
1.3	0	0	5.3	1.1	0	0	4.2	1.8	30	60	1.1	60	60	6.6712892627E - 3	6.6035172472E - 3
1.5	0	0	7.6	1.3	0	0	3.2	0.9	45	108	0.7	120	180	2.99057431511E - 1	2.99065465003E - 1
1.8	0	0	2.7	1.2	0	0	7.3	0.5	135	108	0.3	100	180	5.86131016003E - 1	5.8573726096E - 1
2	0	0	7.6	1	0	0	3.4	2.1	108	300	1.4	60	180	4.27245235718E - 2	4.274584963E - 2
2	1	0	9.4	2	1	0	6.7	2.2	30	45	1.2	60	36	9.91265419036E - 5	9.6780655244E - 5
2.1	1	0	5.8	2.2	0	0	3.7	0.2	105	45	0.5	120	30	-2.307460518359E - 1	-2.30614140417E - 1
3	1	0	7.6	1	0	0	3.4	0.2	108	30	0.4	60	45	4.91667625231E - 1	4.91268324946E - 1
3	1	0	8.8	3	0	0	7.9	0.8	45	45	0.3	120	60	-4.470146899767E - 1	-4.46962329953E - 1

Here $I_{n^*lm,\mu\nu\sigma}(\zeta, \zeta', R_{ab})$ is the two-center nuclear attraction integral over NISTOs determined by [32]

$$\begin{aligned} & I_{n^*lm,n^*l'm'}(\zeta, \zeta', \vec{R}_{ab}) \\ &= \int \chi_{n^*lm}^*(\zeta, \vec{r}_a) \frac{1}{r_b} \chi_{n^*l'm'}(\zeta', \vec{r}_a) dV. \end{aligned} \quad (8)$$

In order to calculate the two-center nuclear attraction integrals we use the Laplace expansion of Coulomb potential. Then we find the following analytical expression for the two-center nuclear attraction integrals:

$$\begin{aligned} & I_{n^*lm,n^*l'm'}(\zeta, \zeta', \vec{R}_{ab}) = (1+t)^{n^*+1/2} (1-t)^{n'^*+1/2} \\ & \cdot \sum_{L=|l-l'|}^{l+l'} \sum_{M=-L}^L \frac{z\sqrt{4\pi}}{(2L+1)^{1/2}} \sqrt{\frac{1}{\Gamma(2n^*+1)\Gamma(2n'^*+1)}} \\ & \times C^{L|M|}(lm, l'm') A_{mm'}^M \\ & \cdot \frac{1}{(2p)^{L+1}} \left[\Gamma(n^* + n'^* + L + 1) \right. \\ & \left. - \Gamma(n^* + n'^* + L + 1, 2p) \right] \\ & + (2p)^{2L+1} \Gamma(n^* + n'^* - L, 2p) \Big] S_{LM}(\theta, \varphi); \end{aligned} \quad (9)$$

here $z = \zeta + \zeta'$, $p = zR/2$, and $t = (\zeta - \zeta')/(\zeta + \zeta')$. See Appendix for exact formulas of $C^{L|M|}(lm, l'm')$, $A_{mm'}^M$ and $S_{lm}(\theta, \varphi)$ quantities and functions occurring in (9). The quantities $\Gamma(\alpha)$ and $\Gamma(\alpha, x)$ in (9) are well-known complete and incomplete gamma functions defined by, respectively,

$$\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} e^{-t} dt, \quad (10)$$

$$\Gamma(\alpha, x) = \int_x^\infty t^{\alpha-1} e^{-t} dt. \quad (11)$$

These functions have already been investigated by numerous authors with different algorithms (see, e.g., [33, 34] and references therein).

As can be seen from (7) and (9), by the use of Guseinov one-range addition theorems, the SF three-center nuclear attraction integrals are expressed through the two-center

TABLE 2: Convergence of the series expansion relations for noninteger SF three-center nuclear attraction integrals over STOs as a function of summation limits for N . $R_{ac} = 1.8$, $\theta_{ac} = 30$, $\phi_{ac} = 60$, $R_{ab} = 1.1$, $\theta_{ab} = 60$, $\phi_{ab} = 60$, and $\alpha = 0$.

N	Eq. (7) for $I_{1,300,1,100}(1.3, 0.7, \vec{R}_{ca}, \vec{R}_{ab})$
5	0.336896384834373
6	0.339487682453034
7	0.340270532993467
8	0.340116042929251
9	0.339661315498115
10	0.339243752352591
11	0.338980006668039
12	0.338868607202027
13	0.338861299222622
14	0.338908803548408
15	0.338971794137852
16	0.339028513191853
17	0.339068958094987
18	0.339092542090420
19	0.339102386725724
20	0.339103160558990

overlap integrals, gamma functions, auxiliary functions, and coefficients. The obtained formula is basic and valid for arbitrary integer and noninteger principal quantum numbers.

4. Numerical Results and Discussion

We have presented a new analytical method for the calculation of self-friction three-center nuclear attraction integrals over STOs and NISTOs with the help of Guseinov one-range addition theorems. The computer programs of established formulas have been performed by using Mathematica 7.0 programming language in Intel (R) Core (TM) 2.5 GHz computer. On the basis of (7), the calculation results of SF three-center nuclear attraction integrals over STOs and NISTOs have been given in Tables 1, 2, and 3. In Table 1, for $\alpha = 0$ and $\alpha = 1$, the comparison results of SF three-center nuclear attraction integrals over STOs and NISTOs have been presented. As can be seen from Table 1 our calculation results are satisfactory. Also, for different values of self-friction quantum number α , the convergence of the series expansion

TABLE 3: Convergence of the series expansion relations for non-integer SF three-center nuclear attraction integrals over STOs as a function of summation limits for N . $R_{ac} = 1.8$, $\theta_{ac} = 30$, $\phi_{ac} = 60$, $R_{ab} = 1.1$, $\theta_{ab} = 60$, $\phi_{ab} = 60$, and $\alpha = 1$.

N	Eq. (7) for $I_{1,300,1,100}(1.3, 0.7, \vec{R}_{ca}, \vec{R}_{ab})$
5	0.34020570374536
6	0.34023045324266
7	0.33972836080133
8	0.33926825347282
9	0.33899764955237
10	0.33890266956856
11	0.33891035305428
12	0.33896166770645
13	0.33901588628170
14	0.33905691933072
15	0.33908024198451
16	0.33909004101075
17	0.33909111299376
18	0.33908862095281
19	0.33908529189431
20	0.33908278090016

relations of $I_{1,300,1,100}(\zeta, \zeta', \vec{R}_{ca}, \vec{R}_{ab})$ SF three-center nuclear attraction integral over NISTOs as a function of summation limits of N had been shown in Tables 2 and 3.

The coefficients $F_m(n)$, $\omega_{mn'}^l$, and $S_{n^*lm,\mu\nu\sigma}(\zeta, \zeta'; \vec{R})$ are repeatedly needed in a computation of the three-center nuclear attraction integrals. We believe that a common storage scheme for the $F_m(n)$ and $\omega_{mn'}^l$ coefficients and $S_{n^*lm,\mu\nu\sigma}(\zeta, \zeta'; \vec{R})$ overlap integrals with the same selection rule, as proposed in this study, will give important contributions in reducing requirements of computer time for computation of multicenter integrals which arise in the Hartree-Fock-Roothaan and Hylleraas approaches. For quick calculations, the $F_m(n)$ and $\omega_{mn'}^l$ coefficients and $S_{n^*lm,\mu\nu\sigma}(\zeta, \zeta'; \vec{R})$ integrals are stored in the memory of the computer. In order to put these coefficients and integrals into or to get them back from the memory, the positions of certain coefficients $F_m(n)$, $\omega_{mn'}^l$, and $S_{n^*lm,\mu\nu\sigma}(\zeta, \zeta'; \vec{R})$ integrals are determined by the following relations.

For $F_m(n)$ binomial coefficients

$$F(n, m) = \frac{n(n+1)}{2} + m + 1. \quad (12)$$

For $\omega_{mn'}^l$ coefficients

$$f_{mn'l} = \frac{1}{6}n(n+1)(n-1) + \frac{1}{2}n'(n'-1) + l + 1. \quad (13)$$

For $S_{n^*lm,\mu\nu\sigma}(\zeta, \zeta'; \vec{R})$ overlap integrals

$$F_{nlm} = \frac{1}{6}n(n-1)(2n-1) + l(l+1) + m + 1. \quad (14)$$

To demonstrate the effectiveness of storage method for given coefficients and integrals we calculated three-center nuclear attraction integral with noninteger quantum numbers. The computer time required for the calculation of three-center nuclear attraction integrals is not given in the tables

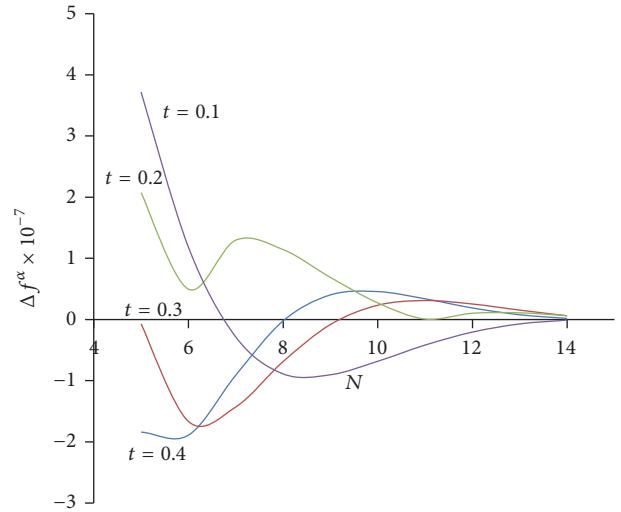


FIGURE 1: The convergence of series in (7) for $\alpha = 0$ with different values of parameter t for noninteger SF three-center nuclear attraction integrals $I_{1,300,1,100}(\zeta, \zeta', \vec{R}_{ca}, \vec{R}_{ab})$ in atomic units (a.u.) as a function of the indices N ($R_{ac} = 1.8$, $\theta_{ac} = 30$, $\phi_{ac} = 60$, $R_{ab} = 1.1$, $\theta_{ab} = 60$, $\phi_{ab} = 60$, and $\alpha = 0$).

due to the fact that the comparison cannot be made with the different computers used in the literature. For instance, for $I_{2,311,2,501}(4.6, 7.2, \vec{R}_{ca}, \vec{R}_{ab})$ with sets $R_{ca} = 0.2$, $\theta_{ca} = \pi/3$, $\phi_{ca} = 2\pi/3$, $R_{ab} = 0.5$, $\theta_{ab} = \pi/4$, $\phi_{ab} = 5\pi/6$, $\alpha = 0$, and $N = 15$ CPU time takes about 5.897 ms and 2.57 ms by using usual and storage methods, respectively.

In Figure 1 we plot the convergence of the series (see (7)) of $I_{1,300,1,100}(\zeta, \zeta', \vec{R}_{ca}, \vec{R}_{ab})$ for $\alpha = 0$ with different values of parameter t as a function of the indices N . The series accuracy $\Delta f^\alpha = f_N^\alpha - f_L^\alpha$ is shown in Figure 1 where the quantities f_L^α are the values of integral for $L < N = N'$. As can be seen from Figure 1, for given α , the convergence rates are satisfactory for arbitrary values of parameter t . Greater accuracy is attainable by the use of more terms of expansions (7).

5. Conclusion

In conclusion, by considering self-friction effects, we have proposed an analytical efficient method for the calculation of three-center nuclear attraction integrals over STOs and NISTOs using Guseinov one-range addition theorems. This allows us to take into account the self-friction field effect in atomic and molecular electronic structure evaluations.

Appendix

The generalized Gaunt coefficients $C^{|\sigma|}(lm, l'm')$ and $A_{mm'}^\sigma$ occurring in (9) are determined by the following relationships [32]:

$$C^{L|M|}(lm, l'm')$$

$$= \begin{cases} C^L(lm, l'm') & \text{for } |M| = |m - m'| \\ C^L(lm, l' - m') & \text{for } |M| = |m + m'|, \end{cases} \quad (A.1)$$

where

$$\begin{aligned}
 C^L(lm, l'm') &= (-1)^{g-(l'-m')+(1/2)(|m|+|m'|+|m-m'|)} \frac{F_g(l+l') F_{g-l}(L)}{(2g+1) F_g(2g) F_l(l+l')} \\
 &\times \left[\frac{(2l+1)(2l'+1) F_l(l+|m|) F_{l'}(|l'+|m'|) F_L(L+|m-m'|)}{F_{|m|}(l) F_{|m'|}(l') F_{|m-m'|}(L)} \right]^{1/2} \\
 &\times \sum_t (-1)^t F_{L-|m-m'|-t}(l'+L-m-t) F_t(l+m+t) F_{l-m-t}(l+l'-L), \\
 A_{mm'}^M &= \begin{cases} \frac{1}{\sqrt{2}} \left(2 - |\eta_{mm'}^{m+m'}| \right)^{1/2} \delta_{M,\varepsilon|m-m'|} + \frac{1}{\sqrt{2}} \eta_{mm'}^{m+m'} \delta_{M,\varepsilon|m+m'|} & \text{for real STOs} \\ \delta_{M,m-m'} & \text{for complex STOs.} \end{cases} \tag{A.2}
 \end{aligned}$$

See [32] for the exact definition of quantities $\eta_{mm'}^{m+m'}$ and $\varepsilon = \varepsilon_{mm'}$.

In this work $S_{lm}(\theta, \varphi)$ is the complex ($S_{lm} \equiv Y_{lm}$) or real spherical harmonics. The definition of phases for the complex spherical harmonics ($Y_{lm}^* = Y_{l-m}$) differs from the Condon-Shortley phases [27] by the sign factor $(-1)^m$ and can be defined as

$$S_{lm}(\theta, \varphi) = P_{l|m|}(\cos \theta) \Phi_m(\phi), \tag{A.3}$$

where

$$\begin{aligned}
 \Phi_m(\phi) &= \frac{1}{\sqrt{\pi(1+\delta_{m0})}} \begin{cases} \cos |m| \phi & \text{for } m \geq 0 \\ \sin |m| \phi & \text{for } m < 0, \end{cases} \\
 P_{l\lambda}(x) &= \frac{(1-x^2)^{\lambda/2}}{2^l} \left[\frac{2l+1}{2F_\lambda(l) F_\lambda(2l)} \right]^{1/2} \sum_{k=0}^{l-\lambda} (-1)^k \\
 &\cdot F_k(\lambda+k) F_{l-k}(2l-2k) F_{l-\lambda-2k}(l-k) x^{l-\lambda-2k}. \tag{A.4}
 \end{aligned}$$

Here $\lambda = |m|$ and $0 \leq k \leq (1/2)\{l-\lambda-(1/2)[1-(-1)^{l-\lambda}]\}$.

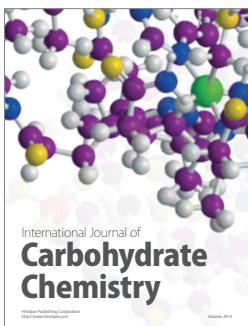
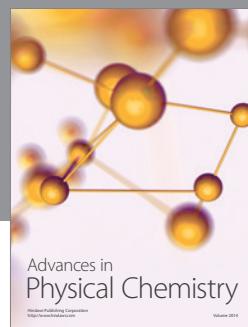
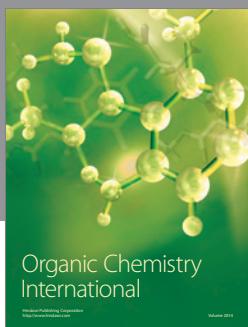
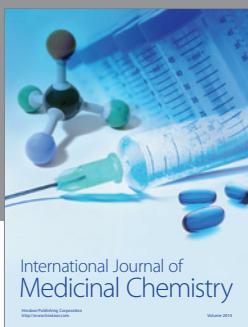
Competing Interests

The author declares that they have no competing interests.

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