

Interaction Between Two Closed Shell Atoms

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Abstract We use the theory of Boehm-Yaris and Jacobi-Csanak to calculate the dipole-dipole, dipole-quadrupole, quadrupole-dipole and quadrupole-quadrupole contributions to the dispersion energy between two different closed shell atoms. To this energy we add one of the Born-Meyer type corresponding to valence effects. In this way we find a finite total interaction energy for any interatomic distance, whose asymptotic behavior reproduces the usual dispersion energy. The results are compared to experimental data and to some theoretical values found in the literature.

1. INTRODUCTION

The interaction potential between atoms and/or molecules is of fundamental importance to understand several static and dynamic properties in gases, liquids and solids¹.

Since the pioneer work of Slater in 1928², a number of simplified potentials have been suggested³⁻²⁶, mainly based on asymptotic solutions of the Schrödinger equation.

In more recent papers one has tried to obtain reliable *universal* formulae for the intermolecular potential in certain gas types, mostly by means of *ab initio* calculations. Particularly Barkan²⁶ suggested recently that the Kiara potential, with carefully calculated parameters, yields a self-consistent description of several macroscopic properties of inert gases.

Even though it is artificial, it is convenient to divide the interaction potential into two types: short range potential (also called

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valence or chemical potential) and long range potential (or Van der Waals potential).

For two closed shell atoms separated by a distance R , the valence potential can be expressed by the ultra-simplified form (Born-Meyer type)

$$V_{\text{val}}(R) = A e^{-bR} \quad (1)$$

where A and b are characteristic parameters of the atomic pair under study.

The long range interaction between two non-polar systems in their respective ground states (as in the case of this paper) is characterized by a dispersion (sometimes called London) potential. This potential is due to the correlation between electrons in distinct atoms. Here the expansion of the inverse internuclear distance (R^{-1}) forms a problematic detail]. Second order perturbation theory, by means of a multipolar expansion, gives for the dispersion potential between two atoms the expansion²⁷

$$V(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \dots \quad (2)$$

where the coefficient C_6 represents the dipole-dipole interaction, C_8 the dipole-quadrupole interaction and C_{10} refers to the quadrupole-quadrupole and dipole-octupole interactions.

From eq. (2) it follows that $V(R) \rightarrow -\infty$ when $R \rightarrow 0$. Nevertheless, it is generally desirable to obtain damped potentials for intermediate and small values of R . Several authors have already treated the damping of interaction dispersion for decreasing values of R . Buckingham and Corner⁷ were the first to work in this direction multiplying the dispersion terms by a damping function dependent on R . Later, Musher and Amos²⁸, introducing terms formed by multiplying polynomials by exponential functions, obtained convergent dispersion series.

More recently, analytical formulae were proposed for the damping of the London potential in ground state atoms. The first of them supplies explicitly the principal term of the dispersion potential between two identical atoms and was published by Jacobi and Csanak²⁹. The technique introduced by those authors is of basic importance for the

present paper and will be discussed in the following section. Richardson³⁰ proposed a completely different technique supplying analytical results for the dipole-dipole, dipole-quadrupole and quadrupole-quadrupole contributions to the dispersion interaction between two atoms. This is a semi-classical formulation where every atom is treated as a harmonic oscillator. Koide³¹, too, introduced a method supplying a convergent series for the dispersion energy. In this method physical properties of every atom appear separately. Koide studied particularly the H_2 system, obtaining analytical formulae for the dipole-dipole and dipole-quadrupole contributions, in the interaction dispersion. The Koide expansion is valid only for spherically symmetrical systems and is nearly equivalent to that of Jacobi-Csanak. Finally, Battezzati and Magnasco³², also, developed an analytical formula for the dispersion energy by a method inspired in works by Longuet-Higgins³³ and McWeeny³⁴. For the dipole-dipole contribution the results obtained in references 32 and 29 are coincident.

2. THE JACOBICSANAK TECHNIQUE

This technique represents essentially an improvement introduced by these authors to that part of the second quantization formalism of Boehm and Yaris³⁵ treating the dispersion energy. This formalism describes the interaction between two systems by a linear response theory based on the many body Green's function techniques of Martin and Schwinger³⁶. Instead of using a multipolar expansion leading to eq. (2), Jacobi and Csanak adopted the strategy of introducing in the formalism of Boehm and Yaris the analytical representation of the Born amplitudes obtained by Csanak and Taylor³⁷.

The basic equation of the work by Jacobi-Csanak can be written in the form

$$V(R) = - \frac{1}{2\pi^5} \sum_L \left[(2\ell_1+1)(2\ell_2+1)(\ell_1\ell_2L;000)^2 \times \sum_{n_1, n_2} g_{n_1\ell_1, n_2\ell_2} I_{n_1\ell_1, n_2\ell_2}^{(L,L)}(R) \right] \quad (3)$$

where $(\ell_1\ell_2L;000)$ are Clebsch-Gordan coefficients,

$$g_{n_1 \ell_1, n_2 \ell_2} = \int_0^\infty du \left[\frac{W_{n_1 \ell_1}}{W_{n_1 \ell_1}^2 + u^2} \cdot \frac{W_{n_2 \ell_2}}{W_{n_2 \ell_2}^2 + u^2} \right] \quad (4)$$

($W_{n\ell}$ = excitation energy)

and

$$I \begin{matrix} (L, L') \\ (R) \\ n_1 \ell_1, n_2 \ell_2 \end{matrix} = \quad (5)$$

$$= \int dq' j_L(q'R) F_{n_1 \ell_1}(q') F_{n_2 \ell_2}(q') \int dq j_L(qR) F_{n_1 \ell_1}^*(q) F_{n_2 \ell_2}^*(q) .$$

In eq. (5) $F_{n\ell}(q)$ is the *radial* part of a Born amplitude which, for an atomic system, can be factorized in the form³⁷

$$F_{\vec{n}}(\vec{q}) = F_{n\ell}(q) Y_{\ell m}(\hat{q}) \quad (6)$$

with $Y_{\ell m}(\hat{q})$ denoting a spherical harmonic of order ℓ and

$$F_{n\ell}(q) = 4\pi i^\ell \sum_{j=1}^N \int \psi_{\vec{n}}^*(X) j_\ell(qr_j) Y_{\ell m}(\hat{r}_j) \psi_{\vec{0}}(X) d\tau . \quad (7)$$

In eq. (7) $\psi_{\vec{n}}$ and $\psi_{\vec{0}}$ are, respectively, the wave functions of the excited and ground states of an atom with N electrons and \vec{q} the momentum absorbed by it during the excitation process. By $X = (x_1, x_2, \dots, x_j, \dots, x_N)$ we are denoting the set of coordinates of the N electrons. $\vec{r}_j = (\vec{r}_j, \omega_j)$ refers to the four coordinates of the j -th electron, three spatial (\vec{r}_j) and one of spin (ω_j). \vec{n} and $\vec{0}$ indicate the set of quantum numbers respectively defining the excited and ground states. The *integration* ranges over all the atomic coordinates (including summing over the spin coordinates) and $d\tau$ is the volume element.

We will adopt the Jacobi-Csanak approximation²⁹, replacing the exact Born amplitudes [eq.(7)] by simplified forms of the corresponding series of Csanak-Taylor³⁷. We refer to the expressions (in atomic unities):

$$F_{n_1}(q) = \alpha^6 D_n \frac{q}{(q^2 + \alpha^2)^3} \quad (8)$$

and

$$F_{n^2}(q) = \frac{1}{2} \alpha^8 Q_n \frac{q^2}{(q^2 + \alpha^2)^4} \quad , \quad (9)$$

where

$$D_n = i \frac{4\pi}{3} \sum_{j=1}^N \int \psi_n^*(X) r_j Y_{10}(\hat{r}_j) \psi_0(X) d\tau \quad , \quad (10)$$

$$Q_n = - \frac{8\pi}{15} \sum_{j=1}^N \int \psi_n^*(X) r_j^2 Y_{20}(\hat{r}_j) \psi_0(X) d\tau \quad (11)$$

and³⁸

$$\alpha = \sqrt{2I} + \sqrt{2(I-W)} \quad . \quad (12)$$

In eq. (12) I is the ionization energy and W one excitation energy.

Equation (3) was applied by its authors only in the calculation of the principal term ($l_1=l_2=1$) of the Van der Waals potential between two helium atoms, separated by intermediate and large (relative to the atomic diameter) distances. It was used also by J.C. Antonio^{3,9} to calculate the dipole-quadrupole term of the dispersion potential between two helium atoms.

3. DISPERSION INTERACTION BETWEEN TWO DIFFERENT CLOSED-SHELL ATOMS

a) Introductory considerations

We will use equations (3), (8) and (9) to obtain analytical expressions for the dipole-dipole, dipole-quadrupole, quadrupole-dipole and quadrupole-quadrupole terms of the dispersion potential between two different closed shell atoms. In particular we will numerically calculate the interaction between an helium atom and neon one. We think that this work is a fair generalization of the calculation made by Jacobi-Csanak^{2,9} and J.C. Antonio³, mainly because our study of the interaction between two distinct atoms demanded an analytical calculation, with very little aid of tables, of quite complex integrals (see Appendix).

We express the dispersion energy in the form

$$V(R) = V_{d,d}(R) + V_{d,q}(R) + V_{q,d}(R) + V_{q,q}(R) \quad (13)$$

and calculate each of these four contributions separately

b) Dipole-dipole contribution

Taking in eq. (3) $\ell_1 = \ell_2 = 1$ and considering that the Clebsch-Gordan coefficients $(\ell_1 \ell_2 L; 000)$ are different from zero only if the conditions $|\ell_1 - \ell_2| \leq L \leq (\ell_1 + \ell_2)$ and $(\ell_1 + \ell_2 + L) = \text{even number}$ are simultaneous fulfilled, we will have

$$V_{d,d}(R) = -\frac{3}{2\pi^5} \sum_{n_1, n_2} g_{n_1, 1, n_2, 1} \left[I_{n_1, 1, n_2, 1}(R) + 2 I_{n_1, 1, n_2, 1}^{(2,2)}(R) \right] \quad (14)$$

Assuming the approximation²⁹ indicated in eqs. (8) and (9) where, for each one of the systems ① and ②, the parameter a defined by (12) is independent of the principal quantum number n , introducing (8) in (5) (with $L = L' = 0$ and $L = L' = 2$) and substituting the results into eq. (14), we obtain

$$V_{d,d}(R) = -\frac{3}{8\pi^3} (\alpha_1 \alpha_2)^{12} \left[\sum_{n_1, n_2} g_{n_1, 1, n_2, 1} |D_{n_1}|^2 |D_{n_2}|^2 \right] \times \left[(Z_{33}^{02}(R))^2 + 2(Z_{33}^{22}(R))^2 \right] \quad (15)$$

where

$$Z_{mn}^{rs}(R; \alpha_1, \alpha_2) = \frac{2}{\pi} \int_0^\infty dq j_r(qR) \frac{q^s}{(q^2 + \alpha_1^2)^m (q^2 + \alpha_2^2)^n} \quad (16)$$

On the other hand, defining the oscillator strength in an atom (in a.u.) as⁴⁰

$$f_{n\ell} = \frac{8\pi}{(2\ell+1)} W_{n\ell} |\langle \psi_n | \sum_{j=1}^N r_j^\ell Y_{\ell 0}(\hat{r}_j) | \psi_0 \rangle|^2 \quad (17)$$

and comparing with eq. (10), we have

$$|D_n|^2 = \frac{2\pi}{3} \frac{f_{n1}}{W_{n1}} \quad (18)$$

So, from eqs. (4) and (18) it follows that

$$\sum_{n_1, n_2} g_{n_1, 1, n_2, 1} |D_{n_1}|^2 |D_{n_2}|^2 = \left(\frac{2\pi}{3}\right)^2 \int_0^\infty du \left\{ \sum_{n_1} \frac{f_{n_1, 1}}{W_{n_1, 1}^2 + u^2} \sum_{n_2} \frac{f_{n_2, 1}}{W_{n_2, 1}^2 + u^2} \right\}.$$

Therefore, defining the dynamic polarizabilities in an atom as⁴⁰

$$\alpha_\ell^{(k)}(\omega) = \sum_{n_k} \frac{f_{n_k, \ell}}{W_{n_k, \ell}^2 - \omega^2} \quad (19)$$

and the dispersion coefficients C_{ℓ_1, ℓ_2} as²¹,

$$C_{\ell_1, \ell_2} = \frac{(2\ell_1 + 2\ell_2)!}{4(2\ell_1)!(2\ell_2)!} \frac{2}{\pi} \int_0^\infty du \alpha_{\ell_1}^{(1)}(iu) \alpha_{\ell_2}^{(2)}(iu) \quad (20)$$

eq. (15) takes the form

$$V_{\vec{d}, \vec{d}}(R) = -\frac{C_{1,1}}{18} (\alpha_1 \alpha_2)^{1,2} \left[(Z_{33}^{0,2}(R))^2 + 2(Z_{33}^{2,2}(R))^2 \right], \quad (21)$$

where C is obtained through eq. (20).

c) Dipole-quadrupole contribution

Taking in eq. (3) $\ell_1 = 1$ and $\ell_2 = 2$ and considering that $(1\ 2L; 0\ 0\ 0)$ is different from zero only for $L = 1$ and $L = 3$ we obtain

$$V_{\vec{d}, \vec{q}}(R) = -\frac{3}{2\pi^5} \sum_{n_1, n_2} g_{n_1, 1, n_2, 2} \left\{ 2 I_{n_1, 1, n_2, 2}^{(1,1)}(R) + 3 I_{n_1, 1, n_2, 2}^{(3,3)}(R) \right\}. \quad (22)$$

Now, introducing eqs. (8) and (9) in eq.(5) (with $L = L' = 1$ and $L = L' = 3$) and substituting the results into eq. (22) we have

$$V_{\vec{d}, \vec{q}}(R) = -\frac{3}{32\pi^3} \alpha_1^{1,2} \alpha_2^{1,6} \left\{ \sum_{n_1, n_2} g_{n_1, 1, n_2, 2} |D_{n_1}|^2 |D_{n_2}|^2 \right\} \times \left[2(Z_{34}^{1,3}(R))^2 + 3(Z_{34}^{3,3}(R))^2 \right], \quad (23)$$

where the $Z_{mm}^{rs}(R)$ are functions to be obtained from eq. (16).

On the other hand from eqs.(11) and (17) we obtain

$$|Q_n|^2 = \frac{8\pi}{45} \frac{f_{n2}}{W_{n2}} \quad (24)$$

Further, from eqs. (4), (18) and (24) it follows that

$$\sum_{n_1, n_2} g_{n_1, 1, n_2, 2} |D_{n_1}|^2 |Q_{n_2}|^2 = \frac{16\pi^2}{135} \int_0^\infty du \left\{ \sum_{n_1} \frac{f_{n_1, 1}}{W_{n_1, 1}^2 + u^2} \sum_{n_2} \frac{f_{n_2, 2}}{W_{n_2, 2}^2 + u^2} \right\}. \quad (25)$$

Finally, using relations (19) and (20) successively in (25) and introducing the result thus obtained in (23), we have

$$V_{d,q}(R) = - \frac{C_{1,2}}{675} \alpha_1^{12} \alpha_2^{16} \left\{ 2(Z_{34}^{13}(R))^2 + 3(Z_{34}^{33}(R))^2 \right\}. \quad (26)$$

d) Quadrupole-dipole contribution

Taking in eq.(3) $\ell_1 = 2$ and $\ell_2 = 1$ and performing the same stages as we did in the preceding sub-section, we find

$$V_{q,d}(R) = - \frac{C_{2,1}}{675} \alpha_1^{16} \alpha_2^{12} \left\{ 2(Z_{43}^{13}(R))^2 + 3(Z_{43}^{33}(R))^2 \right\}, \quad (27)$$

where the coefficient $C_{2,1}$ is calculated through eq.(20) and the parameters α_k ($k = 1, 2$) are obtained through equation (12). The functions $Z_{43}^{13}(R)$ and $Z_{43}^{33}(R)$ result from two of the integrations indicated in eq. (16).

e) Quadrupole-quadrupole contribution

Taking in eq.(3) $\ell_1 = \ell_2 = 2$ and using the procedures and definitions of sub-sections b) and c), we obtain

$$V_{q,q}(R) = - \frac{C_{2,2}}{28350} (\alpha_1 \alpha_2)^{16} \left\{ (Z_{44}^{04}(R))^2 + \frac{10}{7} (Z_{44}^{24}(R))^2 + \frac{18}{7} (Z_{44}^{44}(R))^2 \right\}. \quad (28)$$

f) Results

Introducing eq.(A18) in eqs. (21), (26), (27) and (28) and substituting the results thus obtained into eq.(13), the usual dispersion energy $W(R)$ is reproduced

$$V(R) \xrightarrow{R \rightarrow \infty} - \left\{ \frac{C_{1,1}}{R^6} + \frac{C_{1,2}}{R^8} + \frac{C_{2,1}}{R^8} + \frac{C_{2,2}}{R^{10}} \right\} \equiv W(R) . \quad (29)$$

On the other side, adding the valence energy given by eq.(1) to our dispersion energy [eq.(13)] we obtain the total interaction energy

$$V_{\text{tot}}(R) = V(R) + A e^{-bR} . \quad (30)$$

For a numerical application we choose the He-Ne system, for which $A = 57.00$ a.u. and $b = 2.43$ a.u.²¹. As dispersion coefficients we use those of reference 27, that is, $C_{1,1} = 3.13$ a.u., $C_{1,2} = 17.5$ a.u., $C_{2,1} = 15.2$ a.u and $C_{2,2} = 15.7$ a.u..

In figures 1 and 2 we show a summary of our results, together with equivalent results obtained by other authors. As for the helium atom we first take $\alpha_1 = 1.67508$ a.u. (corresponding with the $1^1S \rightarrow 3^1P$ transition) and subsequently $\alpha_1 = 2.48535$ a.u. (corresponding with the average energy excitation calculated by Victor et al.⁴¹). As for the neon atom we remain with the transitions $(1s)^2 (2s)^2 (2p)^6 (1S_0) \rightarrow 3s^1 (\frac{1}{2})_1^0 (1P_1)$, corresponding to $a = 1.84720$ a.u..

4. ANALYSIS OF THE RESULTS

Our equations and graphs show that:

- a) In the asymptotic region ($R > 4.0 \text{ \AA}$) our results reproduce the usual dispersion energy, being therefore practically independent from the parameters a_1 and a_2 .
- b) In the intermediate region ($2.0 \text{ \AA} < R \leq 4.0 \text{ \AA}$) our curves decrease quite more slowly than in the corresponding usual dispersion energy graph. In this way the dependence of our results relative to a_1 and a_2 does not remain negligible any longer. The shift becomes more pronounced as R becomes smaller. (See in fig. 1 the region $R \leq 4.0 \text{ \AA}$).

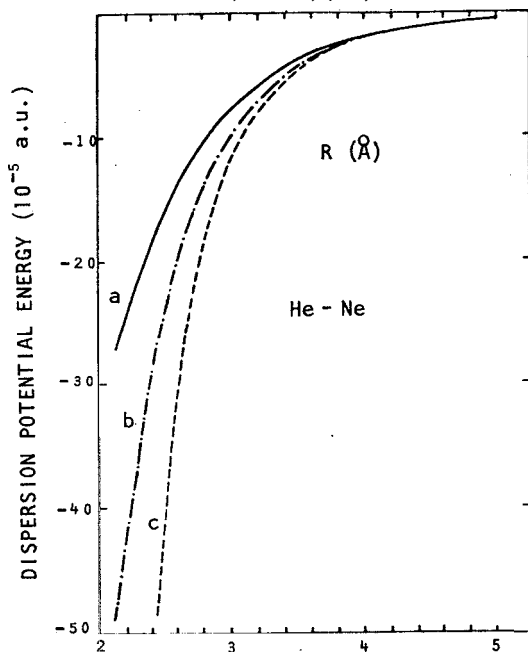


Fig.1 - (a) our dispersion energy for $\alpha_1 = 1.67508$ a.u. and $\alpha_2 = 1.84720$ a.u.; (b) our dispersion energy for $\alpha_1 = 2.48535$ a.u. and $\alpha_2 = 1.84720$ a.u.; (c) usual dispersion energy [eq.(29)].

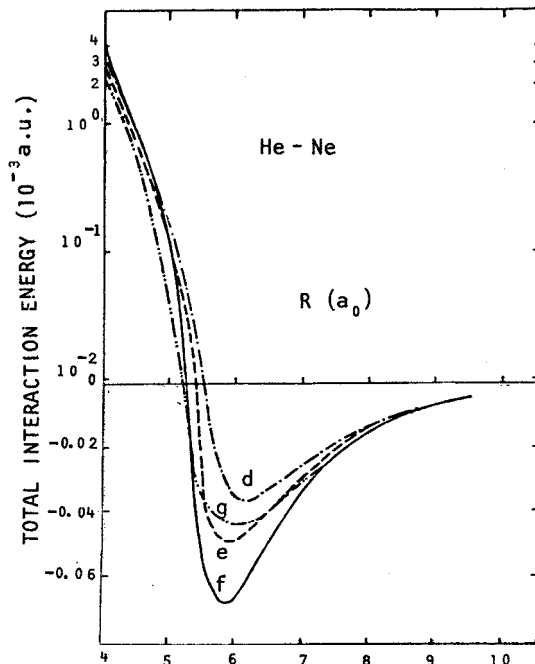


Fig.2 - (d) total interaction energy for $A = 57.0$ a.u., $b = 2.43$ a.u., $\alpha_1 = 1.67508$ a.u. and $\alpha_2 = 1.84720$ a.u. ($a_0 = 0.529$ Å); (e) the same as in (d) for $\alpha_1 = 2.48535$ a.u. and $\alpha_2 = 1.84720$ a.u.; (f) total interaction energy calculated for Rae^{42} ; (g) experimental results of by Chen *et al.*⁴³

- c) Our total interaction energy, given in eq. (30), shows a good agreement with the theoretical work of Rae^{4,2} and with the experimental results of Chen *et al*^{4,3} (see fig.2). It is interesting to see that in the problematic region of the Van der Waals minimum our calculations show a better agreement with the experimental data than Rae's results. Further, it is simple to obtain still better results choosing adequate values for the parameters α_1 and α_2 .
- d) Our results, differently from the usual dispersion energy, do not diverge for small R-values. In this way, they may be useful in the study of problems such as atom-atom scattering.

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APPENDIX - INTEGRALS $Z_{mn}^{rs}(R; \alpha_1, \alpha_2)$

To illustrate the analytical technique used in calculating the integrals Z_{mn}^{rs} defined by eq. (16) let us take

$$Z_{33}^{02}(R; \alpha_1, \alpha_2) = \frac{2}{\pi} \int_0^\infty dq j_0(qR) \frac{q^2}{(q^2 + \alpha_1^2)^3 (q^2 + \alpha_2^2)^3} \quad (A1)$$

As

$$j_0(qR) = \frac{\text{sen}(qR)}{qR}$$

$$Z_{33}^{02}(R; \alpha_1, \alpha_2) = -\frac{1}{R} \frac{dI(R)}{dR} \quad (A2)$$

with

$$I(R) = \frac{2}{\pi} \int_0^\infty dq \frac{\cos(qR)}{(q^2 + \alpha_1^2)^3 (q^2 + \alpha_2^2)^3} \quad (A3)$$

In eq. (A3) the integrand is an even function; so

$$I(R) = \frac{1}{\pi} \int_{-\infty}^{\infty} dq \frac{\cos(qR)}{(q^2 + \alpha_1^2)^3 (q^2 + \alpha_2^2)^3} = \frac{1}{2\pi} \left[\int_{-\infty}^{\infty} dq \frac{e^{iqR}}{(q^2 + \alpha_1^2)^3 (q^2 + \alpha_2^2)^3} + \int_{-\infty}^{\infty} dq \frac{e^{-iqR}}{(q^2 + \alpha_1^2)^3 (q^2 + \alpha_2^2)^3} \right] = \frac{1}{\pi} \int_{-\infty}^{\infty} dq \frac{e^{iqR}}{(q^2 + \alpha_1^2)^3 (q^2 + \alpha_2^2)^3} \quad (A4)$$

The integral (A4) can be calculated with the help of residue theory. To do that let us define the functions $f(z)$ of a complex variable z as follows.

Consider the functions

$$f(z) = \frac{e^{iRz}}{(z^2 + \alpha_1^2)^3 (z^2 + \alpha_2^2)^3} = \frac{e^{iRz}}{(z - i\alpha_1)^3 (z + i\alpha_1)^3 (z - i\alpha_2)^3 (z + i\alpha_2)^3} \quad (A5)$$

and use the contour shown in fig. A1.

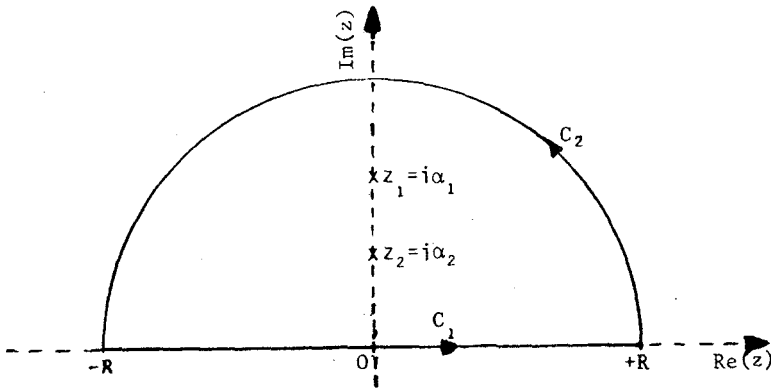


Fig.A1 - Contour to be used in the calculation of integral (A4).

According to the residue theory

$$\oint f(z) dz = \int_{-R}^R f(q) dq + \int_{C_2} f(z) dz = 2\pi i (R_1 + R_2) \quad (A6)$$

where R_1 and R_2 are the residues of the poles of $f(z)$ lying within the integration contour (see fig. A1). We know that those residues are given by

$$R_k = \frac{1}{(m-1)!} \frac{d^{m-1}}{dz^{m-1}} \left[(z-z_k)^m f(z) \right]_{z=z_k}, \quad (k = 1, 2) \quad (A7)$$

where m is the pole's order. In the limit $R \rightarrow \infty$, $\int_{C_2} f(z) dz \rightarrow 0$ and so

$$I(R) = \frac{1}{\pi} \int_{-\infty}^{\infty} f(q) dq = 2i R_1 + 2i R_2 \quad (A8)$$

From eqs. (A5) and (A7) it follows (for $m = 3$) that

$$2i R_1 = -e^{-\alpha_1 R} \left[\frac{R^2}{8 \alpha_1^3 (\alpha_1^2 - \alpha_2^2)^3} + \frac{3R}{8 \alpha_1^4 (\alpha_1^2 - \alpha_2^2)^3} + \frac{3R}{2 \alpha_1^2 (\alpha_1^2 - \alpha_2^2)^4} \right. \\ \left. + \frac{3}{8 \alpha_1^5 (\alpha_1^2 - \alpha_2^2)^3} + \frac{3}{2 \alpha_1^3 (\alpha_1^2 - \alpha_2^2)^4} + \frac{6}{\alpha_1 (\alpha_1^2 - \alpha_2^2)^5} \right]$$

and

$$2i R_2 = -e^{-\alpha_2 R} \left[-\frac{R^2}{8 \alpha_2^5 (\alpha_1^2 - \alpha_2^2)^3} - \frac{3R}{8 \alpha_2^4 (\alpha_1^2 - \alpha_2^2)^4} + \frac{3R}{2 \alpha_2^2 (\alpha_1^2 - \alpha_2^2)^4} \right. \\ \left. - \frac{3}{8 \alpha_2^5 (\alpha_1^2 - \alpha_2^2)^3} + \frac{3}{2 \alpha_2^3 (\alpha_1^2 - \alpha_2^2)^4} - \frac{6}{\alpha_2 (\alpha_1^2 - \alpha_2^2)^5} \right]$$

Applying these two results in eq. (A8) and executing the operations shown in eq. (A2) we obtain:

$$Z_{33}^{02}(R) = - \left\{ \left[P_1(R) + P_3(R) \right] e^{-\alpha_1 R} + \left[P_2(R) - P_3(R) \right] e^{-\alpha_2 R} \right\} \quad (A9)$$

where

$$P_1(R) = E_{110} + E_{111} R, \quad P_2(R) = E_{112} + E_{113} R \quad \text{and} \quad P_3(R) = \frac{6}{(\alpha_1^2 - \alpha_2^2)^5 R},$$

with

$$E_{110} = \frac{1.5}{\alpha_1 (\alpha_1^2 - \alpha_2^2)^4} + \frac{1}{8 \alpha_1^3 (\alpha_1^2 - \alpha_2^2)^3}, \quad E_{111} = \frac{1}{8 \alpha_1^2 (\alpha_1^2 - \alpha_2^2)^3},$$

$$E_{112} = \frac{1.5}{\alpha_2 (\alpha_1^2 - \alpha_2^2)^4} - \frac{1}{8\alpha_2^3 (\alpha_1^2 - \alpha_2^2)^3} \quad \text{and} \quad E_{113} = - \frac{1}{8\alpha_2^2 (\alpha_1^2 - \alpha_2^2)^3}$$

By an direct generalisation of this method we obtain the following results for the remaining integrals pointed out in eqs. (21), (26), (27) and (28). We have

$$Z_{33}^{22}(R) = \frac{1}{\alpha_1 \alpha_2} \left\{ \frac{3}{\alpha_2} + \left[P_4(R) - P_6(R) \right] e^{-\alpha_1 R} + \left[P_5(R) + P_6(R) \right] e^{-\alpha_2 R} \right\}, \tag{A10}$$

where

$$P_4(R) = E_{114} (1 + \alpha_1 R + \frac{1}{2} \alpha_1^2 R^2) + E_{115} R^3 + E_{116} R^4,$$

$$P_5(R) = E_{117} (1 + \alpha_2 R + \frac{1}{2} \alpha_2^2 R^2) + E_{118} R^3 + E_{119} R^4$$

and

$$P_6(R) = \frac{3R^2}{(\alpha_1^2 - \alpha_2^2)^5},$$

with

$$E_{114} = \frac{3}{\alpha_1^6 (\alpha_1^2 - \alpha_2^2)^3} + \frac{9}{\alpha_1^4 (\alpha_1^2 - \alpha_2^2)^4} + \frac{18}{\alpha_1^2 (\alpha_1^2 - \alpha_2^2)^5},$$

$$E_{115} = \frac{0.5}{\alpha_1^3 (\alpha_1^2 - \alpha_2^2)^3} + \frac{1.5}{\alpha_1 (\alpha_1^2 - \alpha_2^2)^4},$$

$$E_{116} = \frac{1}{8\alpha_1^2 (\alpha_1^2 - \alpha_2^2)^3},$$

$$E_{117} = - \frac{3}{\alpha_2^6 (\alpha_1^2 - \alpha_2^2)^3} + \frac{9}{\alpha_2^4 (\alpha_1^2 - \alpha_2^2)^4} - \frac{18}{\alpha_2^2 (\alpha_1^2 - \alpha_2^2)^5},$$

$$E_{118} = - \frac{0.5}{\alpha_2^3 (\alpha_1^2 - \alpha_2^2)^3} + \frac{1.5}{\alpha_2 (\alpha_1^2 - \alpha_2^2)^4}$$

and

$$E_{119} = - \frac{1}{8\alpha_2^2 (\alpha_1^2 - \alpha_2^2)^3}$$

We have

$$Z_{34}^{13}(R) = \left[P_7(R) + P_9(R) \right] e^{-\alpha_1 R} + \left[P_8(R) - P_{10}(R) \right] e^{-\alpha_2 R}, \quad (A11)$$

where

$$P_7(R) = E_{120} + E_{121} R, \quad P_8(R) = E_{122} + E_{123} R + E_{124} R^2,$$

$$P_9(R) = \frac{10(1 + \alpha_1 R)}{(\alpha_1^2 - \alpha_2^2)^6 R^2} \quad \text{and} \quad P_{10}(R) = \frac{10(1 + \alpha_2 R)}{(\alpha_1^2 - \alpha_2^2)^6 R^2},$$

with

$$E_{120} = 2/(\alpha_1^2 - \alpha_2^2)^5, \quad E_{121} = \frac{1}{8\alpha_1(\alpha_1^2 - \alpha_2^2)^4}, \quad E_{122} = 3/(\alpha_1^2 - \alpha_2^2)^5,$$

$$E_{123} = \frac{1}{48\alpha_2^3(\alpha_1^2 - \alpha_2^2)^3} - \frac{3}{8\alpha_2(\alpha_1^2 - \alpha_2^2)^4} \quad \text{and} \quad E_{124} = \frac{1}{48\alpha_2^2(\alpha_1^2 - \alpha_2^2)^3}$$

We have

$$Z_{34}^{33}(R) = -\frac{15}{R^4} \left\{ \frac{1}{\alpha_1^6 \alpha_2^8} + \left[P_{11}(R) - P_{13}(R) \right] e^{-\alpha_1 R} + \left[P_{12}(R) + P_{14}(R) \right] e^{-\alpha_2 R} \right\}, \quad (A12)$$

where

$$P_{11}(R) = E_{125} \left(1 + \alpha_1 R + \frac{1}{2} \alpha_1^2 R^2 + \frac{1}{6} \alpha_1^3 R^3 \right) + E_{126} R^4 + E_{127} R^5,$$

$$P_{12}(R) = E_{128} \left(1 + \alpha_2 R + \frac{1}{2} \alpha_2^2 R^2 + \frac{1}{6} \alpha_2^3 R^3 \right) + E_{129} R^4 + E_{1210} R^5 + E_{1211} R^6,$$

$$P_{13}(R) = (1 + \alpha_1 R) R^2 / (\alpha_1^2 - \alpha_2^2)^6 \quad \text{and} \quad P_{14}(R) = (1 + \alpha_2 R) R^2 / (\alpha_1^2 - \alpha_2^2)^6,$$

with

$$E_{125} = \frac{1}{\alpha_1^6 (\alpha_1^2 - \alpha_2^2)^4} + \frac{4}{\alpha_1^4 (\alpha_1^2 - \alpha_2^2)^5} + \frac{10}{\alpha_1^2 (\alpha_1^2 - \alpha_2^2)^6},$$

$$E_{126} = \frac{1}{24\alpha_1^2(\alpha_1^2 - \alpha_2^2)^4} + \frac{2}{15(\alpha_1^2 - \alpha_2^2)^5}, \quad E_{127} = \frac{1}{120\alpha_1(\alpha_1^2 - \alpha_2^2)^4},$$

$$E_{128} = \frac{1}{\alpha_2^8(\alpha_1^2 - \alpha_2^2)^3} - \frac{3}{\alpha_2^6(\alpha_1^2 - \alpha_2^2)^4} + \frac{6}{\alpha_2^4(\alpha_1^2 - \alpha_2^2)^5} - \frac{10}{\alpha_2^2(\alpha_1^2 - \alpha_2^2)^6},$$

$$E_{129} = \frac{1}{24\alpha_2^4(\alpha_1^2 - \alpha_2^2)^3} - \frac{1}{8\alpha_2^2(\alpha_1^2 - \alpha_2^2)^4} + \frac{1}{5(\alpha_1^2 - \alpha_2^2)^5},$$

$$E_{1210} = \frac{1}{120\alpha_2^3(\alpha_1^2 - \alpha_2^2)^3} - \frac{1}{40\alpha_2(\alpha_1^2 - \alpha_2^2)^4} \quad \text{and} \quad E_{1211} = \frac{1}{720\alpha_2^2(\alpha_1^2 - \alpha_2^2)^3}$$

We have

$$Z_{43}^{13}(R) = - \{ (P_{15}(R) + P_{17}(R)) e^{-\alpha_1 R} + (P_{16}(R) - P_{18}(R)) e^{-\alpha_2 R} \}, \quad (A13)$$

where

$$P_{15}(R) = E_{210} + E_{211}R + E_{212}R^2, \quad P_{16}(R) = E_{213} + E_{214}R,$$

$$P_{17}(R) = \frac{10(1 + \alpha_1 R)}{(\alpha_1^2 - \alpha_2^2)^6 R^2} \quad \text{and} \quad P_{18}(R) = \frac{10(1 + \alpha_2 R)}{(\alpha_1^2 - \alpha_2^2)^6 R^2},$$

with

$$E_{210} = 3/(\alpha_1^2 - \alpha_2^2)^5, \quad E_{211} = \frac{1}{48\alpha_1^3(\alpha_1^2 - \alpha_2^2)^3} + \frac{3}{8\alpha_1(\alpha_1^2 - \alpha_2^2)^4},$$

$$E_{212} = \frac{1}{48\alpha_1^2(\alpha_1^2 - \alpha_2^2)^3}, \quad E_{213} = 2/(\alpha_1^2 - \alpha_2^2)^5 \quad \text{and} \quad E_{214} = -\frac{1}{8\alpha_2(\alpha_1^2 - \alpha_2^2)^4}$$

We have

$$Z_{43}^{33}(R) = - \frac{15}{R^4} \left\{ -\frac{1}{\alpha_1^8 \alpha_2^6} + (P_{19}(R) + P_{21}(R)) e^{-\alpha_1 R} + (P_{20}(R) - P_{22}(R)) e^{-\alpha_2 R} \right\}, \quad (A14)$$

where

$$P_{19}(R) = E_{215} (1 + \alpha_1 R + \frac{1}{2} \alpha_1^2 R^2 + \frac{1}{6} \alpha_1^3 R^3) + E_{216} R^4 + E_{217} R^5 + E_{218} R^6,$$

$$P_{20}(R) = E_{219} (1 + \alpha_2 R + \frac{1}{2} \alpha_2^2 R^2 + \frac{1}{6} \alpha_2^3 R^3) + E_{2110} R^4 + E_{2111} R^5,$$

$$P_{21}(R) = \frac{(1 + \alpha_1 R) R^2}{(\alpha_1^2 - \alpha_2^2)} \quad \text{and} \quad P_{22}(R) = \frac{(1 + \alpha_2 R) R^2}{(\alpha_1^2 - \alpha_2^2)^6},$$

with

$$= - \left[\frac{1}{\alpha_1 (\alpha_1^2 - \alpha_2^2)^2} + \alpha_1^6 (\alpha_1^2 - \alpha_2^2)^{-4} + \alpha_1^4 (\alpha_1^2 - \alpha_2^2)^{-5} + \frac{10}{\alpha_1^2 (\alpha_1^2 - \alpha_2^2)} \right],$$

$$E_{216} = - \left[\frac{1}{24 \alpha_1^4 (\alpha_1^2 - \alpha_2^2)^3} + \frac{1}{8 \alpha_1^2 (\alpha_1^2 - \alpha_2^2)^4} + \frac{1}{5 (\alpha_1^2 - \alpha_2^2)^5} \right],$$

$$E_{217} = - \left[\frac{1}{120 \alpha_1^3 (\alpha_1^2 - \alpha_2^2)^3} + \frac{1}{40 \alpha_1 (\alpha_1^2 - \alpha_2^2)^4} \right], \quad E_{218} = - \frac{1}{720 \alpha_1^2 (\alpha_1^2 - \alpha_2^2)^3}$$

$$E_{219} = \frac{1}{\alpha_2^6 (\alpha_1^2 - \alpha_2^2)^4} - \frac{4}{\alpha_2^4 (\alpha_1^2 - \alpha_2^2)^5} + \frac{10}{\alpha_2^2 (\alpha_1^2 - \alpha_2^2)^6},$$

$$E_{2110} = \frac{1}{24 \alpha_2^2 (\alpha_1^2 - \alpha_2^2)^4} - \frac{2}{15 (\alpha_1^2 - \alpha_2^2)^5} \quad \text{and} \quad E_{2111} = \frac{1}{120 \alpha_2 (\alpha_1^2 - \alpha_2^2)^4}.$$

We have

$$Z_{44}^{04}(R) = - \left\{ (P_{23}(R) + P_{25}(R)) e^{-\alpha_1 R} + (P_{24}(R) - P_{25}(R)) e^{-\alpha_2 R} \right\},$$

(A15)

where

$$P_{23}(R) = E_{220} + E_{221}R + E_{222}R^2, \quad P_{24}(R) = E_{223} + E_{224}R + E_{225}R^2$$

and

$$P_{25}(R) = \frac{10(\alpha_1^2 + \alpha_2^2)}{(\alpha_1^2 - \alpha_2^2)^7 R},$$

with

$$E_{220} = -\frac{1}{16\alpha_1^3(\alpha_1^2 - \alpha_2^2)^4} - \frac{1.5}{\alpha_1(\alpha_1^2 - \alpha_2^2)^5} + \frac{5\alpha_1}{(\alpha_1^2 - \alpha_2^2)^6},$$

$$E_{221} = -\frac{1}{16\alpha_1^2(\alpha_1^2 - \alpha_2^2)^4} + \frac{0.5}{(\alpha_1^2 - \alpha_2^2)^5}, \quad E_{222} = \frac{1}{48\alpha_1(\alpha_1^2 - \alpha_2^2)^4},$$

$$E_{223} = -\frac{1}{16\alpha_2^3(\alpha_1^2 - \alpha_2^2)^4} + \frac{1.5}{\alpha_2(\alpha_1^2 - \alpha_2^2)^5} + \frac{5\alpha_2}{(\alpha_1^2 - \alpha_2^2)^6},$$

$$E_{224} = -\frac{1}{16\alpha_2^2(\alpha_1^2 - \alpha_2^2)^4} - \frac{0.5}{(\alpha_1^2 - \alpha_2^2)^5} \quad \text{and} \quad E_{225} = \frac{1}{48\alpha_2(\alpha_1^2 - \alpha_2^2)^4}$$

We have

$$Z_{44}^{24}(R) = \frac{1}{R^3} \{ (P_{26}(R) - P_{28}(R))e^{-\alpha_1 R} + (P_{27}(R) + P_{28}(R))e^{-\alpha_2 R} \}, \quad (A16)$$

where

$$P_{26}(R) = E_{226}(1 + \alpha_1 R + \frac{1}{2}\alpha_1^2 R^2) + E_{227}R^3 + E_{228}R^4 + E_{229}R^5,$$

$$P_{27}(R) = E_{2210}(1 + \alpha_2 R + \frac{1}{2}\alpha_2^2 R^2) + E_{2211}R^3 + E_{2212}R^4 + E_{2213}R^5$$

and

$$P_{28}(R) = \frac{5(\alpha_1^2 + \alpha_2^2)R^2}{(\alpha_1^2 - \alpha_2^2)^7},$$

with

$$\begin{aligned}
 E_{226} &= 60/(\alpha_1^2 - \alpha_2^2)^7, \quad E_{227} = 5\alpha_1/(\alpha_1^2 - \alpha_2^2)^6, \\
 E_{228} &= 0.5/(\alpha_1^2 - \alpha_2^2)^5, \quad E_{229} = \frac{1}{48\alpha_1(\alpha_1^2 - \alpha_2^2)^4}, \\
 E_{2210} &= -60/(\alpha_1^2 - \alpha_2^2)^7, \quad E_{2211} = 5\alpha_2/(\alpha_1^2 - \alpha_2^2)^6, \\
 E_{2212} &= -0.5/(\alpha_1^2 - \alpha_2^2)^5 \text{ and } E_{2213} = \frac{1}{48\alpha_2(\alpha_1^2 - \alpha_2^2)^4}
 \end{aligned}$$

Finally we have

$$Z_{44}^{44}(R) = -\frac{105}{R^5} \left\{ -\frac{1}{\alpha_1^8 \alpha_2^8} + (P_{29}(R) - P_{31}(R))e^{-\alpha_1 R} + (P_{30}(R) + P_{32}(R))e^{-\alpha_2 R} \right\}, \tag{A17}$$

where

$$P_{29}(R) = E_{2214} \left(1 + \alpha_1 R + \frac{1}{2} \alpha_1^2 R^2 + \frac{1}{6} \alpha_1^3 R^3 + \frac{1}{24} \alpha_1^4 R^4 \right) + E_{2215} R^5 + E_{2216} R^6 + E_{2217} R^7,$$

$$P_{30}(R) = E_{2218} \left(1 + \alpha_2 R + \frac{1}{2} \alpha_2^2 R^2 + \frac{1}{6} \alpha_2^3 R^3 + \frac{1}{24} \alpha_2^4 R^4 \right) + E_{2219} R^5 + E_{2220} R^6 + E_{2221} R^7,$$

$$P_{31}(R) = \frac{(150 + 150\alpha_1 R + (67.5\alpha_1^2 + 3.75(\alpha_1^2 - \alpha_2^2))R^2)R^2}{105(\alpha_1^2 - \alpha_2^2)^7}$$

and

$$P_{32}(R) = \frac{(150 + 150\alpha_2 R + (67.5\alpha_2^2 - 3.75(\alpha_1^2 - \alpha_2^2))R^2)R^2}{105(\alpha_1^2 - \alpha_2^2)^7},$$

with

$$E_{2214} = \frac{1}{\alpha_1^8(\alpha_1^2 - \alpha_2^2)^4} + \frac{4}{\alpha_1^6(\alpha_1^2 - \alpha_2^2)^5} + \frac{10}{\alpha_1^4(\alpha_1^2 - \alpha_2^2)^6} + \frac{20}{\alpha_1^2(\alpha_1^2 - \alpha_2^2)^7},$$

$$E_{2215} = \left(\frac{7}{8\alpha_1^3 (\alpha_1^2 - \alpha_2^2)^4} + \frac{3.5}{\alpha_1 (\alpha_1^2 - \alpha_2^2)^5} + \frac{5\alpha_1}{(\alpha_1^2 - \alpha_2^2)^6} \right) \frac{1}{105} ,$$

$$E_{2216} = \left(\frac{7}{48\alpha_1^2 (\alpha_1^2 - \alpha_2^2)^4} + \frac{0.5}{(\alpha_1^2 - \alpha_2^2)^5} \right) \frac{1}{105} , \quad E_{2217} = \frac{1}{5040\alpha_1 (\alpha_1^2 - \alpha_2^2)^4} ,$$

$$E_{2218} = \frac{1}{\alpha_2^8 (\alpha_1^2 - \alpha_2^2)^4} - \frac{4}{\alpha_2^6 (\alpha_1^2 - \alpha_2^2)^5} + \frac{10}{\alpha_2^4 (\alpha_1^2 - \alpha_2^2)^6} - \frac{20}{\alpha_2^2 (\alpha_1^2 - \alpha_2^2)^7} ,$$

$$E_{2219} = \left(\frac{7}{8\alpha_2^3 (\alpha_1^2 - \alpha_2^2)^4} - \frac{3.5}{\alpha_2 (\alpha_1^2 - \alpha_2^2)^5} + \frac{5\alpha_2}{(\alpha_1^2 - \alpha_2^2)^6} \right) \cdot \frac{1}{105} ,$$

$$E_{2220} = \frac{1}{105} \left(\frac{7}{48\alpha_2^2 (\alpha_1^2 - \alpha_2^2)^4} - \frac{0.5}{(\alpha_1^2 - \alpha_2^2)^5} \right) \text{ and } E_{2221} = \frac{1}{5040\alpha_2 (\alpha_1^2 - \alpha_2^2)^4} .$$

It is interesting to note that the functions (A9) - (A17) are analytical and that, for large values of R, we have the following behavior

$$Z_{33}^{02} \rightarrow 0 , \quad Z_{33}^{22} \rightarrow \frac{3}{(\alpha_1 \alpha_2)^6} \frac{1}{R^3} , \quad Z_{34}^{13} \rightarrow 0 , \quad Z_{34}^{33} \rightarrow \frac{15}{\alpha_1^6 \alpha_2^8} \frac{1}{R^4} , \quad Z_{43}^{13} \rightarrow 0 ,$$

$$Z_{43}^{33} \rightarrow \frac{15}{\alpha_1^8 \alpha_2^6} \frac{1}{R^4} , \quad Z_{44}^{04} \rightarrow 0 , \quad Z_{44}^{24} \rightarrow 0 \text{ and } Z_{44}^{44} \rightarrow \frac{105}{(\alpha_1 \alpha_2)^8} \frac{1}{R^5} .$$

(A18)

REFERENCES

1. J.O.Hirschfelder, C.F.Curtiss and R.B.Bird, *Molecular Theory of Gases and Liquids*, Wiley, New York (1954).
2. J.C.Slater, Phys. Rev. 32, 349 (1928).

3. J.C.Slater and J.G.Kirkwood, *Phys. Rev.* 37, 682 (1931).
4. R.A.Buckingham, *Proc. R.Soc.London Ser. A* 168, 264 (1938).
5. H.Margenau, *Phys. Rev.* 56, 1000 (1939).
6. R.Heller, *J.Chem.Phys.* 9, 154 (1941).
7. R.A.Buckingham and J.Corner, *Proc. R. Soc. London Ser. A* 189, 118 (1947).
8. F.C.Brooks, *Phys. Rev.* 86, 92 (1952).
9. A.A.Frost and J.H.Woodson, *J.Am.Chem.Soc.* 80, 2615 (1958).
10. D.Y.Kim, *Z.Phys.* 166, 359 (1962).
11. R.B.Bernstein and F.A.Morse, *J.Chem.Phys.* 40, 917 (1964).
12. V.P.Trubitsyn, *Fiz.Tverd.Tela* 8, 862 (1966) [*Sov.Phys.Solid State* 8, 688 (1966)].
13. L.W.Bruch and I.J.McGee, *J.Chem.Phys.* 46, 2959 (1967).
14. R.K.Nesbet, *J.Chem.Phys.* 48, 1419 (1968).
15. D.D.Konowalow, *J.Chem.Phys.* 50, 12 (1969).
16. D.D.Konowalow and D.S.Zakheim, *J.Chem.Phys.* 57, 4375 (1972).
17. J.P.Toennies, *Chem. Phys. Lett.* 20, 238 (1973).
18. A.F.Wagner, G.Das and A.C.Wahl, *J.Chem.Phys.* 60, 1885 (1974).
19. J.Hepburn, G.Scoles and R.Penco, *Chem.Phys.Lett.* 36, 451 (1975).
20. R.Ahlich, R.Penco and G.Scoles, *Chem.Phys.* 19, 119 (1977).
21. K.T.Tang and J.P.Toennies, *J.Chem.Phys.* 66, 1496 (1977).
22. K.T.Tang and J.P.Toennies, *J.Chem.Phys.* 68, 5501 (1978).
23. K.Ng, W.J.Meath and A.R.Allnat, *Chem.Phys.* 32, 175 (1978).
24. K.Ng, W.J.Meath and A.R.Allnat, *Mol.Phys.* 37, 237 (1979).
25. R.Feltgen, *J.Chem.Phys.* 74(2), 1186 (1981).
26. E.S.Barkan, *Sov.Teach.Phys.* 29(6), 644 (1984).
27. K.T.Tang, J.M. Norbeck and P.R.Certain, *J.Chem.Phys.* 64, 3063 (1976).
28. J.I.Musher and A.T.Amos, *Phys.Rev.* 164, 31 (1967).
29. N.Jacobi and Gy.Csanak, *Chem.Phys.Lett.* 30, 367 (1975).
30. D.D.Richardson, *J.Phys. A* 8, 1828 (1975).
31. A.Koide, *J.Phys. B* 9, 3137 (1976).
32. M.Battezzati and V.Magnasco, *J.Chem.Phys.* 67, 2924 (1977).
33. H.C.Longuet-Higgins, *Proc.R.Soc.London Ser. A* 235, 537 (1956).
34. R.McWeeny, *Rev.Mod.Phys.* 32, 335 (1960).
35. R.Boehm and R.Yaris, *J.Chem.Phys.* 55, 2620 (1971).

36. P.C.Martin and J.S.Schwinger, Phys.Rev. 115, 1342 (1959).
37. Gy. Csanak and H.S.Taylor, Phys.Rev. A6, 1843 (1972).
38. E.N.Lassetre, J.Chem.Phys.43, 4479 (1965).
39. José Carlos Antonio, Tese de Mestrado (instituto de Física e Química da USP, São Carlos, SP (1981)).
40. W.Meyer, Chem. Phys. 17, 27 (1976).
41. G.A.Victor, A.Dalgarno and A.J.Taylor, J.Phys. B1, 13 (1968).
42. A.I.M.Rae, Molecular Physics 29, 467 (1975).
43. C.H.Chen, P.N.Siska and Y.T.Lee, J.Chem.Phys. 59, 601 (1973).

Resumo

O formalismo de Bohem-Yaris e Jacobi-Csanak é usado no cálculo dos termos dipolo-dipolo, dipolo-quadrupolo, quadrupolo-dipolo e quadrupolo-quadrupolo da energia de dispersão entre dois diferentes átomos de camadas fechadas. A esta energia foi adicionada uma energia de valência do tipo Born-Meyer. Assim foi obtida uma energia total de integração finita para todas as distâncias inter-atômicas, cuja forma assintótica reproduz a energia de dispersão usual. Os resultados foram comparados com dados experimentais e outros valores teóricos disponíveis na literatura.