Temperature dependence of the pressure broadening of spectral lines

G D Roston and M S Helmi
Department of Physics, Faculty of Science, Alexandria University, Egypt
E mail: dr.gamal_daniel@yahoo.com

Abstract. The aim of this work is to obtain a formula relating the pressure broadening coefficient of the spectral line $\beta$ with the temperature $T$, when the difference potential $\Delta V(R)$ between the upper and lower states of the emitting atom is represented by (Lennard – Jones) potential, The obtained formula is a power index law of $\beta$ on $T$. This formula is applied for calculating $\beta$ for different interactions of Ar, Ne, TI, Hg, Cd and Zn with the inert gases (Xe, Kr, Ar, Ne and He) at different temperatures. The results of these calculations are in good agreement with the corresponding values obtained before numerically. The obtained formula is considered very important in astrophysical problems.

1. Introduction

In some applications there is a tendency to represent the dependence of the pressure broadening coefficient $\beta = \gamma / N$ on the temperature $T$ in the form of a power law:

$$\beta = T^k$$

where $\gamma$ is the half width of the spectral line and $k$ is the temperature dependence index [1, 2]. $\gamma$ in the impact region is proportional to the density $N$ of the perturbing atoms. The power dependence can be derived theoretically from the classical phase – shift theory of line broadening in the impact limit if the interatomic potentials, $V(R)$ for the upper and lower levels of the emitting atom are approximated by $V(R) = C_p R^{-p}$, where $R$ is the interatomic separation and $C_p$ is a constant. In such a case the impact theory predicts for the index $k$ a formula given by [3]:

$$K = (p - 3) / 2(p - 1)$$

This means that $k$ is dependent only on the power $p$ characterizing the type of interaction. Bielski, et al, [4], obtained the power law dependence of $\beta$ for a Lennard – Jones through the function $B(\alpha)$, which was obtained by Hindmarsh, et al, [5]. The obtained formula by Bielski, et al, [4] didn’t give any explicit form for the power law dependence of $\beta$ on temperature. Moreover, the calculation of $\beta$ in [4] is performed numerically. The authors [6-8] proposed algebraic formulas for the broadening $\rho_b$ and shift $\rho_0$, impact parameters of a spectral line based on the assumption that the ranges of the interaction respectively for the broadening and shift are different. In this work the algebraic formula for the broadening is solved and the broadening coefficient $\beta$ is obtained as a power index law on the temperature $T$.

2. Mathematical treatment

2.1. Power Law Dependence For a Lennard – Jones Potential
If \( V'(R) \) and \( V''(R) \) represent respectively the interaction potentials for the lower and upper states of the emitting atom, are given by Lennard – Jones potential, then the difference potential \( \Delta V(R) = V''(R) - V'(R) \) can be written as

\[
\Delta V(R) = \hbar (\Delta C_{12} R^{-12} - \Delta C_{6} R^{-6})
\]

where \( (\Delta C_{6} \) and \( \Delta C_{12} \)) are respectively the interaction parameters between the colliding particles in case of the long range attractive and repulsive van der Waals potentials. In previous papers [6-8], the authors obtained a formula relating the impact broadening parameter \( \rho_{ob} \) with temperature \( T \) using the potential equation (3) as:

\[
(\alpha_{12} \Delta C_{12} / \sqrt{8K/\pi \mu})\rho_{ob}^{-11} = (\alpha_{6} \Delta C_{6} / \sqrt{8K/\pi \mu})\rho_{ob}^{-5} = 0.63 T^{1/2}
\]

where \( \alpha_{p} \) is a constant depending on the number \( p \) \( (\alpha_{p} = \sqrt{\pi} \Gamma((p - 1)/2)/\Gamma(p/2)) \), and \( \mu \) is the reduced mass between the interacting particles. The parameter \( \rho_{ob} \) is related to the pressure broadening coefficient \( \beta \), and the relative velocity \( v \) in angular frequency unit by the relation:

\[
\beta = \sqrt{\rho_{ob} \pi \mu \alpha \rho \pi \mu} = cT^{K}
\]

\( C \) here is the velocity of light. The first and second terms on the left hand side of equation 4 represent respectively the phase shifts of the broadening \( \eta_p = (\alpha_p C_p / \sqrt{v}) \rho_{ob}^{(p-1)} \) due to the repulsion \( [\Delta C_6 = 0] \) and attraction \( [\Delta C_{12} = 0] \). Comparing equations 1 and 5, and using equation 2 the parameter \( \rho_{ob} \) is related to \( T \) by the relation:

\[
\rho_{ob} = T^{(12k-1)/4} = T^{-1/(2(p-1))}
\]

It is seen from equation 2 that for the long range attractive van der Waals potential \( (p = 6) \) and the pure repulsive form of the potential equation 3 \( (p = 12) \), the temperature index \( k \) are respectively equal to 0.3 and 9/22. These are the cases of equation 6 when the formula 4 is used in its attractive form \( (\Delta C_{12} = 0) \), or in its repulsive form \( (\Delta C_{6} = 0) \).

### 2.2. The Fitting formula

To solve equation (4) for \( \rho_{ob} \), we put:

\[
(\alpha_{12} \Delta C_{12} / \sqrt{8K/\pi \mu})\rho_{ob}^{-11} = A \rho_{ob}^{-11} = x\sqrt{T}
\]

and

\[
(\alpha_{6} \Delta C_{6} / \sqrt{8K/\pi \mu}) \rho_{ob}^{-5} = B \rho_{ob}^{-5} = (x - 0.63)\sqrt{T}
\]

\[
\rho_{ob} = (A / B)^{1/6} (x / (x - 0.63))^{-1/6}
\]

and

\[
T = (B^{1/6} (x^{5/11} / (x - 0.63))^{1/13} = (B^{1/6} / A^{5/13})^{1/3} F_1(x)
\]

\[
F_1(x) = (x^{5/11} / (x - 0.63))^{1/13}
\]

The function \( F_1(x) \) was fitted to the power law of \( X \), so that.

\[
F_1(x) = L_1 x^{-L_1}
\]

The values of the constants \( L_1 \) and \( L_1' \) depend on the ranges of \( x \) as shown in table 1

### Table 1. The Fitting parameters for the two Functions \( F_1(x) \) and \( F_2(x) \) in the different ranges of \( X \)

| Range of X | Values of \( F_1(x) \) | Parameters of \( F_1(x) \) | Values of \( F_2(x) \) | Parameters of \( F_2(x) \) |
|-----------|-----------------------|-----------------------------|-----------------------|-----------------------------|
| From | To | From | To | \( L_1 \) | \( L_1' \) | From | To | \( L_2 \) | \( L_2' \) |
| 0.66 | 0.75 | 191923.71 | 1472.6658 | 0.03 | -36.3 | 122.9636394 | 17.9641291 | 0.238 | -15.03 |
| 0.76 | 1.2 | 1122.6138 | 10643740 | 46.77 | -10.5 | 1646814133 | 213084863 | 4.820 | -4.477 |
| 1.21 | 2.5 | 10125263 | 0.4639603 | 23.96 | -4.53 | 2492365681 | 0.5712784 | 3.670 | -2.03 |
| 2.6 | 10 | 0.4091784 | 0.012695 | 5.06 | -2.64 | 0.580905335 | 0.110253 | 1.940 | -1.262 |
| 10.1 | 25 | 0.0124140 | 0.0017570 | 1.772 | -2.15 | 0.10905300 | 0.041561 | 1.2637 | -0.6727 |
From this, we conclude that, if the temperature \( T \) and the interaction parameters \( \Delta C_6 \) and \( \Delta C_{12} \) are known, then \( F_1(x) \) is obtained and consequently \( x \) from the table 1 and the relation 11. As \( x \) is known, then \( \rho_{ob} \) can be obtained using equation 8, and consequently \( \beta \) from equation 5.

### 2.3. The broadening parameters \( \beta \)

We have from equation 7a

\[
\rho_{ob} = A^{1/11} x^{-1/11} T^{-1/22}
\]

Then equation 5 will take the form

\[
\beta = D \rho_{ob} \sqrt{T} = DA^{2/11} \left[ x^{-4/9} T \right]^{9/22} = DA^{2/11} (T_x)^{9/22}
\]

where

\[
D = \sqrt{\frac{8k}{\pi \mu}} / C
\]

Substituting for \( T \) in \( T_x \) from equation 9, we have

\[
(T_x)^{9/22} = \left[ x^{-4/9} T \right]^{9/22} = B^{1/2} A^{-1/2} \left( x^{1/3} (x - 0.63) \right)^{3/2}
\]

\[
\beta = DB^{3/2} A^{-1/2} \left( x^{1/3} (x - 0.63) \right)^{3/2} = \beta_0 F_2(x)
\]

where

\[
\beta_0 = DB^{3/2} A^{-1/2}
\]

and

\[
F_2(x) = \left( x^{1/3} (x - 0.63) \right)^{3/2}
\]

### 2.4. The relations between the two functions \( F_1(x) \) and \( F_2(x) \)

We have from equation 13

\[
T_x = x^{-4/9} T
\]

We put, instead of \( T \), its expression from equation 9

\[
T_x = x^{-4/9} \left( B^{11} / A^5 \right)^{1/3} F_1(x)
\]

Substituting in equation 13, we have

\[
\beta = DA^{2/11} \left( x^{-4/9} \left( B^{11} / A^5 \right)^{1/3} F_1(x) \right)^{9/22}
\]

\[
\beta = D \left( B^{11} / A^5 \right)^{1/2} x^{-2/11} (F_1(x))^{9/22}
\]

Comparing equations 16 and 22, we have

\[
F_2(x) = x^{-2/11} (F_1(x))^{9/22}
\]

From the fitting formula 11, equation 22 takes the form

\[
F_2(x) = L_{\text{2}}^{9/22} x^{-y/22} (L_1^{4/9} + 4/9) = L_{\text{2}} x^{-L_2^{9/22}}
\]

where

\[
L_2 = L_1^{9/22} \text{ and } L_2' = \left( \frac{9}{22} \right) (L_1' + 4/9)
\]

The values of the constants \( L_2 \) and \( L_2' \) are listed in table 1 depending on the ranges of the values of the function \( F_2(x) \).

### 2.5. The power dependence of \( \beta \) on the temperature \( T \)

From equation 13 we have

\[
\beta = DA^{2/11} x^{-2/11} T^{9/22}
\]

Introducing instead of \( x \), its value from equations (9) and (11), we have

\[
F_1(x) = L_1 x^{-L_1} = B^{-11} A^3 T
\]
corresponding Hindmarsh and Roston and Helmi values with the inert gases (Xe, Kr, Ar, Ne and He). The results are illustrated in the table 2 with the inert gases.

From equation 30, we see that by applying the (L-J) potential, the broadening parameter \( \beta \) is a power law of temperature as in cases when the difference potential \( \Delta(R) \) for the upper and lower levels of the emitting atom is given by \( \Delta(R) = C_p R^\gamma \).

3. Results

The broadening coefficients were calculated for different interactions of Ar, Ne, TI, Hg, Cd and Zn atoms with the inert gases (Xe, Kr, Ar, Ne and He). The results are illustrated in the table 2 with the corresponding Hindmarsh and Roston and Helmi values \( \beta_{ii} \) and \( \beta_{[7,8]} \) with the temperature dependence index \( k = \frac{9}{22} (1 + 4/9L_i^2) \).

### Table 2. The calculated values of pressure broadening coefficient \( \beta \) and \( \beta_0 \) with the corresponding Hindmarsh values \( \beta_{ii} \) and \( \beta_{[7,8]} \) in units \( 10^{-20} \text{ cm}^2/\text{atom cm}^3 \) for Ar, Ne, TI, Hg, Cd and Zn perturbed by inert gases. \( \Delta C_6 \) in units \( 10^{-12} \text{ cm}^2 \text{ rad s}^{-1} \) and \( \Delta C_{12} \) in units \( 10^{-34} \text{ cm}^12 \text{ rad s}^{-1} \) are taken from the labelled references.

| Perturber | \( \Delta C_6 \) | \( \Delta C_{12} \) | \( F_1(X) \) | \( k \) | \( \beta_0 \) | \( \beta \) | \( \beta_{ii} \) | \( \beta_{[7,8]} \) |
|-----------|----------------|----------------|-------------|-----|---------|-------|-----------|-----------------|
| Ar[9]     | 531.8          | 83750          | 20.6022     | 0.4264 | 0.58942 | 6.987 | 7.040     | 6.930           |
| Ne[9]     | 130.0          | 55870          | 2696.02     | 0.4141 | 0.7388  | 8.155 | 8.250     | 8.170           |
| He[9]     | 70.50          | 48190          | 72810.28    | 0.4141 | 1.24391 | 13.73 | 13.89     | 13.75           |
| Ar[10]    | 1114           | 224.8x106      | 329.43      | 0.4264 | 1.1247  | 13.33 | 13.35     | 13.27           |
| Ne[10]    | 2551           | 1011x108       | 8981.11     | 0.4141 | 2.485   | 27.43 | 27.62     | 27.33           |
| He[10]    | 4993           | 2733x109       | 18639.1     | 0.4141 | 4.595   | 50.72 | 50.84     | 50.27           |
| Ar[11]    | 5400           | 12400          | 72480       | 0.4492 | 0.0866  | 1.172 | 1.153     | 1.170           |
| Ar[12]    | 2900           | 88000          | 120.82      | 0.4264 | 0.1557  | 1.846 | 1.870     | 1.870           |
| Ar[13]    | 58.70          | 15.250         | 0.0593      | 0.4779 | 0.05124 | 1.295 | 1.900     | 1.949           |
| Ne[12]    | 14.30          | 6.5800         | 4.6626      | 0.4492 | 0.0864  | 1.798 | 1.640     | 1.800           |
| Ar[14]    | 0.2970         | 0.0010         | 0.6975      | 0.4492 | 0.0089  | 0.186 | 0.207     | 0.202           |
| Kr[15]    | 0.7920         | 0.0080         | 0.8218      | 0.4492 | 0.014806 | 416  | 0.308     | 0.314           |
| Ne[16]    | 0.7450         | 0.0640         | 106.08      | 0.4264 | 0.0473  | 0.843 | 0.850     | 0.847           |
| Ar[17]    | 1.3900         | 0.0110         | 0.172       | 0.4779 | 0.0116  | 0.292 | 0.359     | 0.370           |
| Kr[18]    | 0.2190         | 0.0127         | 242.12      | 0.4264 | 0.024   | 0.429 | 0.428     | 0.437           |
| Ar[17]    | 0.2197         | 0.0306         | 1720.8      | 0.4141 | 0.0387  | 0.636 | 0.549     | 0.510           |
| Ne[17]    | 0.3740         | 0.0388         | 616.46      | 0.4264 | 0.0457  | 0.816 | 0.775     | 0.753           |
| He[17]    | 0.3170         | 0.0106         | 576.56      | 0.4264 | 0.0663  | 1.184 | 1.190     | 1.200           |
| Zn[19]    | 1.7875         | 0.0199         | 0.3431      | 0.4779 | 0.0174  | 0.441 | 0.491     | 0.441           |
| Ar[20]    | 0.1650         | 0.0072         | 524.58      | 0.4264 | 0.0290  | 0.518 | 0.514     | 0.515           |
| Ne[21]    | 0.1337         | 0.0030         | 417.99      | 0.4264 | 0.0298  | 0.531 | 0.529     | 0.531           |
4. Conclusions
From the foregoing discussions and relations we conclude the following:

1. If \( T \) and \((\Delta C_6, \Delta C_{12})\) are known, then the broadening parameters \( \beta \) can be obtained using equations 9, 8 and 5.

2. If \( \beta \) and \((\Delta C_6, \Delta C_{12})\) are known, then \( F_2(x) \) is obtained using equation 16, which leads to the function \( F_1(x) \) from equation 24 and then \( T \) using equation 9.

3. If \( \beta \) and \( T \) are known, then \( \Delta C_6 \) and \( \Delta C_{12} \) can be obtained using equations 9 and 16.

4. The broadening parameters \( \beta \) were calculated for different interactions. These calculations are illustrated with the corresponding values of Hindmarsh and the previous work of the authors [7,8] as in table 2. It is seen that our calculating results for \( \beta \) are in good agreement with the values obtained before especially for interactions containing light particles. The discrepancy between the values of \( \beta \) for heavy particles can be attributed to the change of the sign of the phase value \( \pm 0.63 \).

5. The obtained analytical formulas can be used simply to obtain information about the far source parameters “astrophysical problems”.

6. The values of the temperature dependence index \( k \) for all interactions are very near to the value \( 9/22=0.4091 \) when the repulsion part from the potential only is applied.

References
[1] Lwin A, Mc Cartan D D and Levis E L 1977 J. Astrophys. 213 599
[2] Spielfiedel A and Roueff E 1981 J. Phys. B. 14 L795
[3] Peach G 1981 Adv. Phys. 30 367
[4] Bielski A, Bobkowski R, and Szudy J 1989 Astron. Astrophys. 208 357
[5] Hindmarsh W R, Petford A D and Smith G 1967 Proc. Roy. Soc. London. A297 296
[6] Helmi MS 1994 Pak. J. Sci. Ind. Res. 37 12 499
[7] Helmi M S and Roston G D 2000 Physica Scripta 62 36
[8] Roston G D , Ghatass Z F and Obaid F S 2009 JQSRT. 110 175 183
[9] Bielski A, Wawrzynski J and Wolnikowski J 1985. Acta Physica Pol. 67A. 3 621
[10] Wolnikowski J, Wawrzynski J, Bielski A and Szudy J 1987 Physica Scripta 35. 153
[11] Bielski A, Dokurno W, Szudy J and Wolnikowski J 1980 J. Physica B 60. 101C. 113
[12] Dygdala RS 1988 J. Phys. B:At. Mol. Opt. Phys. 21 2039
[13] Dygdala RS, Bobkowski R and Lisicki E J 1989 J. Phys. B:At. Mol. Phys. 22 1563
[14] Czuchaj E, Rebentrost F and Stoll H, Preuss H 1997 Chem.Phys. 214 277
[15] Okunishi M, Nakazawa H, Yamanouchi K and Suchiya S 1990 Revisited. J.Chem.Phys. 93. 7526
[16] Kurosawa T, Ohmori K, Chiba H, Okunishi M, Ueda K and Sato Y 1998 J. Chem. Phys. 108 8101
[17] Czuchaj E. and Stoll H 1999 Chem.Phys. 248 1
[18] Czajkowski M, Bobkowski R and Krause L 1991 Phys Rev A. 44 9 5730
[19] Czajkowski M and Koperski J 1999 Spectrochimica Acta A 55 2221
[20] Inguar Wallace, Jarral Ryter and Breckenridge W H 1992 J. Phys. Chem. 96 882
[21] Koperski J and Czajkowski M 2000 Phys. Rev. A. 62 012505.