Van der Waals Forces between Copper and Noble-Gas Atoms

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(Z. Naturforsch. 30 a, 1203-1204 [1975]; received April 21, 1975)

The Van der Waals constants for the five lowest energy levels of Cu(I) interacting with noble-gas atoms have been calculated using a semiempirical method. A comparison with the values obtained from the Coulomb approximation is presented.

Information on the interatomic potential is essential for the interpretation of many phenomena involving atom-atom collisions. The long range attractive potential between two atoms is usually represented by the Van der Waals potential

$$V(r) = -C_6 r^{-6},$$

where $r$ is the interatomic distance. Although the problem of calculating the constant $C_6$ has been the subject of many investigations, it is known for a few interacting atoms only. Most studies have been done for the interaction between alkali and noble-gas atoms. This note reports the results of semiempirical evaluations of $C_6$ for the five lowest energy levels of copper interacting with noble-gas atoms.

Let us suppose that the atom A (e.g. Cu) is in the state described by the quantum numbers $k, J, M$ ($k = n, L$), and the perturbing atom B (noble-gas atom) is in its ground state $^1S_0$. According to Margenau and Fiutak and Frackowiak, the constant $C_6(kJ,M)$ may be written in the form

$$C_6(kJ,M) = \frac{aI}{2(2J+1)} \sum_{k'J'M'} S(kJ,k'J') \left[ E_{kJ} - E_{k'J'} + I \right] \left[ 1 + 3(1J'M|M) \right]^{1/2} \left[ 1 + 3(1J'0M|M) \right]^{1/2},$$

(2)

where $(1J'M|M)$ denotes the Clebsch-Gordan coefficient and $S(kJ,k'J')$ is the line strength for the $(kJ) \rightarrow (k'J')$ transition.

The matrix elements in Eq. (1) are calculated in a rotating coordinate system where the $z$-axis is parallel to the line connecting the atoms A and B. Equation (1) has been derived from the general expression for $C_6$ assuming that the excitation energy $AE_B$ of the noble gas atoms are nearly equal to the ionization energy $I$ of the atom B. Applying the Eckart-Wigner theorem to the second term in the numerator of Eq. (1) we can transform it to the form

$$C_6(kJ,M) = \frac{aI}{2} \sum_{k'J'M'} \frac{S(kJ,k'J') \left[ E_{kJ} - E_{k'J'} + I \right]}{E_{kJ} - E_{k'J'} + I} \left[ 1 + 3(1J'M|M) \right]^{1/2} \left[ 1 + 3(1J'0M|M) \right]^{1/2},$$

(2)

Table 1. Constants $C_6$ for Cu(I) in units of $10^{-58}$ erg cm$^6$. SE — semiempirical values from Equation (2). CA — values obtained from the Coulomb approximation Equations (4) — (5).

| State      | $| M |$ | He SE | Ne SE | Ar SE | Kr SE | Xe SE |
|------------|-----|-------|-------|-------|-------|-------|
| $3d^{10}4s^2d^1$ | $^2S_{1/2}$ | 1/2 | 0.103 | 0.100 | 0.185 | 0.185 | 0.717 | 0.679 | 1.06 | 0.973 | 1.66 | 1.52 |
| $3d^{10}4s^2d^1$ | $^2P_{1/2}$ | 1/2 | 0.308 | 0.260 | 0.563 | 0.503 | 2.27 | 2.01 | 3.43 | 2.98 | 5.50 | 4.80 |
| $3d^{10}4s^2d^1$ | $^2P_{3/2}$ | 1/2 | 0.407 | 0.323 | 0.746 | 0.624 | 3.01 | 2.51 | 4.56 | 3.74 | 7.33 | 6.04 |
| $3d^{10}4s^2d^1$ | $^2D_{5/2}$ | 3/2 | 0.253 | 0.209 | 0.462 | 0.403 | 1.85 | 1.60 | 2.79 | 2.35 | 4.45 | 3.78 |
| $3d^{10}4s^2d^1$ | $^2D_{3/2}$ | 1/2 | 0.00404 | 0.00733 | 0.0283 | 0.0297 | 0.0429 | 0.0473 | 0.166 | 0.152 |
| $3d^{10}4s^2d^1$ | $^2D_{5/2}$ | 1/2 | 0.00305 | 0.00553 | 0.0216 | 0.0231 | 0.0321 | 0.0505 | 0.0564 | 0.0564 |
| $3d^{10}4s^2d^1$ | $^2D_{3/2}$ | 3/2 | 0.00744 | 0.0134 | 0.0518 | 0.0768 | 0.1199 | 0.1199 |
| $3d^{10}4s^2d^1$ | $^2D_{5/2}$ | 5/2 | 0.00609 | 0.0110 | 0.0424 | 0.0629 | 0.0982 | 0.0982 |
| $3d^{10}4s^2d^1$ | $^2D_{3/2}$ | 7/2 | 0.00319 | 0.00631 | 0.0244 | 0.0361 | 0.0561 | 0.0561 |

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We have calculated the line strengths for CuI from the experimental transition probabilities taken from a recent critical review of existing experimental data. Therefore, in the present study we have calculated the line strengths for CuI using the experimental transition probabilities taken from a recent critical review of existing experimental data. The following five energy levels of CuI from a recent critical review of existing experimental data are shown in Table 1. We have used the following experimental values for noble-gas polarizabilities in units of 10^{-24} cm^3: 0.216 for He, 0.398 for Ne, 1.63 for Ar, 2.48 for Kr, 4.01 for Xe. They do not differ significantly from the theoretical values listed in the paper of Mahan.

The only previously reported data of the constants C_6 for CuI are those of Miyachi and JayaRam for the 3d^{10} 4p^{2}P_{1/2,3/2} levels for the interaction with argon atoms. Their calculations are based on the Mahan method in which a Coulomb approximation of the Bates-Damgaard type is used. In the Coulomb approximation, C_6(nM_L) is given by

\[ C_6(nM_L) = \frac{\beta e^2 a_B^2 a(n^*)^2}{(2L+3)(2L-1)} \]

where \( e \) is the electronic charge, \( a_B \) the Bohr radius, and \( n^* \) the effective quantum number.

The values of the coefficient \( a_{M_L} \) as well as \( C_6(nM_L) \) are listed in the paper of Mahan. In the Coulomb approximation, \( C_6(nL M_L) \) is given by

\[ C_6(nL M_L) = \frac{5(n^*)^2 + 1 - 3L(L + 1) [5L(L + 1) - 3(M_L^2 + 1)]}{(2L+3)(2L-1)} \]

As can be seen in Table 1 there is reasonable agreement between the semiempirical values of the Van der Waals constants with those obtained from the Coulomb approximation we also have calculated using the expressions given by Mahan.

According to Mahan, the constant \( C_6(k J M) \) can be written as the sum of two terms

\[ C_6(k J M) = C_6^{(0)}(k J M) + C_6^{(1)}, \]

where the second term \( C_6^{(1)} \) depends only on the noble-gas atom and the first term \( C_6^{(0)}(k J M) \) is a linear combination of constants \( C_6^{(0)}(n L M_L) \) corresponding to quantum numbers \( nL M_L \):

\[ C_6^{(0)}(k J M) = \sum_{M_L} a_{M_L} C_6^{(0)}(n L M_L). \]