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# BINDING ENERGY OF DIATOMIC MOLECULES USING SCREENED COULOMB POTENTIAL FUNCTION

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Screened Coulomb interaction potential function has been used to study the binding energy of twenty alkali halides and twelve heavy metal halides. The results are compared with their experimental values and other theoretical results.

**Keywords: Binding Energy ; Diatomic Molecule; Potential Energy Function ; Force-Constant**

## INTRODUCTION

THE energy change in the process of transformation of the gaseous molecules to the separated ions is defined as the binding energy of molecules. This has been determined by methods like electron diffraction, microwave spectroscopy and thermochemical processes. Theoretical models (Patel *et al.*, 1967; Varshni & Shukla, 1961; Gohel, 1969; and Pant, 1976) have also been applied to determine it, assuming molecules to be constituted of ions. For earlier developments, reference may be made to Goodisman (1973). In this communication, Screened Coulomb potential energy function has been used to study binding energy of alkali and heavy metal halide molecules, as this form is found to give better results in case of crystals.

## MATERIALS AND METHODS

The binding energy of molecules, $D_i$, which is defined as

$$D_i = -U(r_e) \qquad \ldots(1)$$

can be obtained if the potential energies of molecules are known for equilibrium internuclear distance $r_e$. These can be calculated using Screened Coulomb potential energy function which is given by

$$U(r) = -\frac{e^2}{r} + \frac{b}{r} e^{-\lambda r} \qquad \ldots(2)$$

for diatomic molecules. Here $b$ and $\lambda$ are potential parameters, and $r$ is the distance between the ions of the molecules. Potential parameters are determined through force-constants obtained from molecular spectra. The conditions that determine these are

$$U'(r_e) = 0 \qquad \ldots(3)$$

and

$$U''(r_e) = k_e \qquad \ldots(4)$$

$U'(r_e)$ and $U''(r_e)$ are the first and second derivatives of $U(r)$ at $r = r_e$ the equilibrium internuclear distance. $K_e$ is the force-constant.

## Results and Discussion

Calculated values of potential parameters using equations (2), (3) and (4) are recorded in Tables I and II for alkali halides and heavy metal halides respectively. $r_e$ and $K_e$ needed for the purpose of evaluating parameters $b$ and $\lambda$ are recorded in their respective tables with their sources.

Table I

*Experimental data and potential parameter b and λ for alkali halide molecules*

| Molecule | $r_e$ (Å) Honig *et al.* (1954) | $K_e \times 10^{-5}$ (dyne/cm Thakur (1975) | $\lambda \times 10^{-8}$ ($cm^{-1}$) | $b \times 10^{16}$ (erg cm) |
|---|---|---|---|---|
| LiF | 1.540*a* | 2.4586 | 3.0791 | 0.04667 |
| LiCl | 2.037*a* | 1.4982 | 3.1162 | 0.1787 |
| LiBr | 2.170 | 1.2467 | 2.9443 | 0.1860 |
| LiI | 2.392 | 0.9719 | 2.7742 | 0.2302 |
| NaF | 2.000*a* | 1.4650 | 2.9681 | 0.1259 |
| NaCl | 2.361 | 1.1004 | 3.0305 | 0.3623 |
| NaBr | 2.502 | 0.9582 | 2.9529 | 0.4345 |
| NaI | 2.711 | 0.7627 | 2.7553 | 0.4773 |
| KF | 2.171*b* | 1.2038 | 2.8570 | 0.1641 |
| KCl | 2.667 | 0.8640 | 2.9973 | 0.7601 |
| KBr | 2.821 | 0.7009 | 2.7316 | 0.5886 |
| KI | 3.048 | 0.5264 | 2.4087 | 0.4553 |
| RbF | 2.265*c* | 1.3913 | 3.4861 | 0.6970 |
| RbCl | 2.787 | 0.7666 | 2.9008 | 0.8283 |
| RbBr | 2.945 | 0.6697 | 2.8210 | 1.0056 |
| RbI | 3.177 | 0.4924 | 2.9333 | 0.6017 |
| CsF | 2.345 | 1.4500 | 3.8401 | 1.8656 |
| CsCl | 2.906 | 0.7195 | 2.9418 | 1.2465 |
| CsBr | 3.072 | 0.5675 | 2.6113 | 0.7793 |
| CsI | 3.315 | 0.3897 | 2.1205 | 0.3246 |

*a*—Thakur (1975).
*b*—Green and Lew (1960)
*c*—Lew *et al.* (1958).

Calculated values of binding energies for alkali halides and heavy metal halides are presented in Tables III and IV respectively. For comparison corresponding experimental and some other theoretical values are also recorded in the same table. The experimental values have been estimated through

$$D_i = D_e + I - E \qquad ...(5)$$

where $D_e$, $I$ and $E$ are dissociation energy, ionisation potential and electron affinity and are taken from Gaydon (1953), Pauling (1963) and Wagman *et al.* (1965) respectively.

The agreement between observed and calculated values is good for alkali fluorides except Cesium flouride. Although our values in other cases are close to experimental values, the agreement is not so good as obtained by Rittner who has

TABLE II

*Experimental data and potential parameter b and λ for heavy metal halides*

| Molecule | $r_e$ (Å) Barrett & Mandel (1958) | $K_e \times 10^{-5}$ (Dyne/cm) Gohel (1969) | $\lambda \times 10^{-8}$ ($cm^{-1}$) | $b \times 10^{16}$ (erg. cm) |
|---|---|---|---|---|
| TlF | 2.0844 | 2.310 | 4.7842 | 4.5244 |
| TlCl | 2.4848 | 1.453 | 4.2565 | 7.8166 |
| TlBr | 2.6181 | 1.763 | 5.5954 | 399.2267 |
| TlI | 2.8135 | 1.037 | 3.9426 | 13.6627 |
| InCl | 2.4011 | 1.586 | 4.3435 | 6.8297 |
| InBr | 2.5432 | 1.366 | 4.1890 | 8.3871 |
| InI | 2.7539 | 1.114 | 3.9948 | 11.5238 |
| GaCl | 2.2017 | 1.952 | 4.5142 | 4.3692 |
| GaBr | 2.3525 | 1.516 | 4.1251 | 3.5334 |
| GaI | 2.5747 | 1.212 | 3.8935 | 4.7256 |
| CuCl | 2.0500 | 2.284 | 4.6018 | 2.7643 |
| CuI | 2.3340 | 1.734 | 4.4860 | 7.0911 |

TABLE III

*Binding energy, $D_1$, of alkali halides in kcal/mole*

| Molecule | Estimated | Present study | Theoretical (Varshni & Shukla, 1961) | | |
|---|---|---|---|---|---|
| | | | B. M. | Rittner | Varshni & Shukla |
| LiF | 177.6 | 177.68 | 178.8 | 185.8 | 184.0 |
| LiCl | 151.3 | 141.03 | — | — | — |
| LiBr | 141.8 | 132.47 | 132.7 | 142.1 | 132.7 |
| LiI | 132.8 | 120.70 | 127.0 | 130.6 | 123.0 |
| NaF | 141.7 | 142.20 | — | — | — |
| NaCl | 128.0 | 123.68 | 123.7 | 130.0 | 125.5 |
| NaBr | 123.4 | 117.33 | 117.2 | 127.7 | 118.8 |
| NaI | 106.5 | 108.07 | 108.3 | 118.9 | 109 8 |
| KF | 131.3 | 131.98 | 132.2 | 136.5 | 134.7 |
| KCl | 113.4 | 110.76 | 110.9 | 116.2 | 112.2 |
| KBr | 108.1 | 104.46 | 104.4 | 109.5 | 105.8 |
| KI | 103.9 | 95.92 | 96.1 | 101.1 | 97.5 |
| RbF | 135.6 | 130.26 | 130.1 | 135.7 | 131.8 |
| RbCl | 111.3 | 106.10 | 106.2 | 111.4 | 107.5 |
| RbBr | 105.8 | 100.73 | 100.8 | 106.4 | 102.0 |
| RbI | 100.8 | 92.61 | 92.7 | 97.6 | 94.0 |
| CsF | 133.0 | 127.60 | 127.6 | 135.4 | 128.9 |
| CsCl | 107.7 | 102.35 | 102.5 | 108.1 | 103.6 |
| CsBr | 102.2 | 96.16 | 96.3 | 101.3 | 97.5 |
| CsI | 95.2 | 87.74 | 84.4 | 88.3 | 85.4 |

TABLE IV

*Binding energy of heavy metal halides in kcal/mole*

| Molecules | Estimated | Present study | Rittner's form (Gohel, 1969) | B. L. form (Pant, 1976) | B. M. form (Pant, 1969) |
|---|---|---|---|---|---|
| TlF | 151.3 | 145.55 | 159.2 | 142.78 | 140.94 |
| TlCl | 135.3 | 112.17 | 132.3 | 121.11 | 122.11 |
| TlBr | 127.7 | 118.80 | 180.8 | 121.49 | 123.00 |
| TlI | 121.7 | 107.44 | 127.4 | 107.02 | 108.42 |
| InCl | 134.9 | 126.26 | 155.9 | 124.45 | 125.83 |
| InBr | 124.3 | 119.43 | 138.6 | 125.60 | 126.93 |
| InI | 118.3 | 110.59 | 130.0 | 137.42 | 113.22 |
| GaCl | 160.5 | 137.26 | 156.0 | 135.42 | 136.79 |
| GaBr | 131.9 | 128.03 | 145.9 | 126.00 | 127.41 |
| GaI | 125.9 | 117.33 | 124.5 | 115.91 | 117.06 |
| CuCl | 170.5 | 146.17 | — | 144.40 | 146.12 |
| CuI | 144.9 | 129.93 | — | 128.40 | 129.59 |

considered other interactions such as charge induced dipole, induced dipoleinduced-dipole, Van der Waals attraction and thermal energy of vibration etc.

In case of heavy metal halides, the values Calculated here are equally good as those of others by exponential Born-Mayer's form or Rittner's form.

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