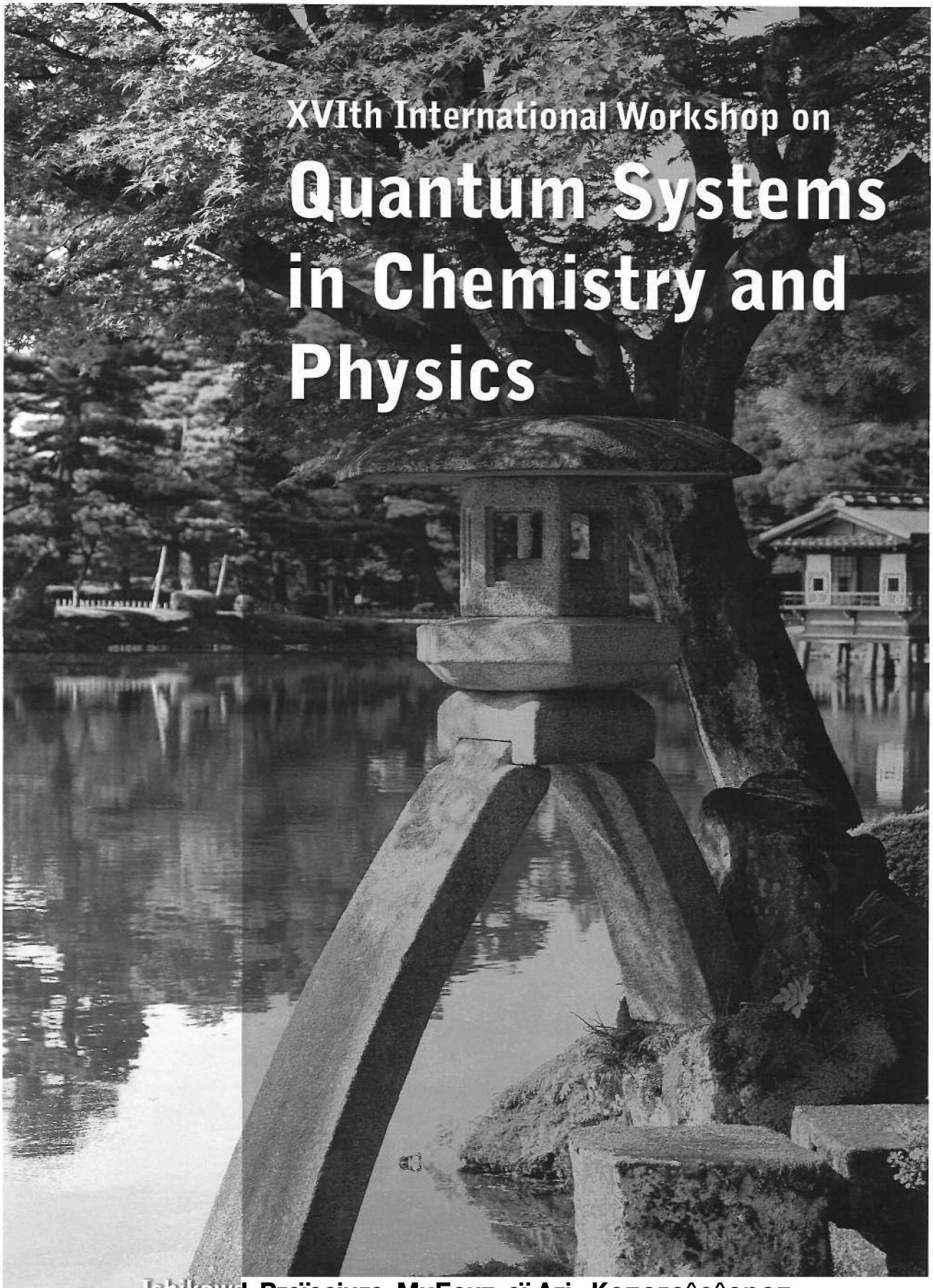

Ishikawa Рreïесіиге МиБеит оїАгі, Капага^а^арап

Determination of Atomic Charges in Molecules and Ions

Valentin Oshchapovsky
Lviv State University of Vital Activity Safety 35 Kleparivska Str., Lviv, 79007, Ukraine

A new method of calculation of the lattice energy of binary ionic crystals of MX type was developed [1]. It enabled to deduce a new universal formula for the lattice energy calculation taking into account only ion radii values without introducing any additional arbitrary factors. It is pointed out that the exactness of Ulat calculation depends upon the ionnity bond degree [1]. The above-mentioned allowed deducting an equation for a priori calculation of the length of interatomic distances in crystals and gaseous molecules assuming that all the bonds are of pure ionic type [2]. Furthermore, the equation for the calculation of ion radii with an arbitrary effective charge was deduced [3]. The ion radii in the binary non-polar molecules of halogens, chalcogens etc. were calculated: e.g., $R^{IV}(F^{+}) = 0.255$ A, $R^{IV}(Br^{+}) = 0.918$ A, $R^{IV}(At^{+}) = 1.147$ A .

On the basis of these values, during the use of the previously received equation for a priori determination of interatomic distances [2] there were calculated Rl2 values for the large group of molecules of different type: halogens, interhalogenides, chalcogens, nitrogens and their combinations. It allowed to solve a reverse side of the problem i.e., to estimate the atomic charges of the large group of binary gaseous molecules according to the value of intemuclear distance: I_2 ($0^{192+}0^{K92}$), NI ($C^{176+}C^{l7<"}$), $C0_2$ ($C^{368+}0^{184"}$), N_2 ($N^{269+}N^{269}$l, NO ($N^{187+}0'^{87}$), $N0_2$ ($N^{383+}0'^{915}$). Considering the experimental Rl2 values there were also calculated the values of atomic charges in the ionized molecules, e.g. I_2^{+} ($O^{287+}0'^{87"}$) and I_2 ($O^{097+}O^{l97}$). The radius of He^{+} ion was calculated. The possibility of estimation of ion co-ordination, bond multiplicity as well as some correction of ion radii R sizes is shown.

1. Oshchapovskii V.V. Russian J. of General Chemistry, 2008, V.78, No. 4, p.532-542.
2. Oshchapovskii V.V. Russian J. of Inorganic Chemistry, 2010, V.55, No. 3, p. 401-409.
3. Oshchapovskii V.V. Russian J. of Inorganic Chemistry (in press).