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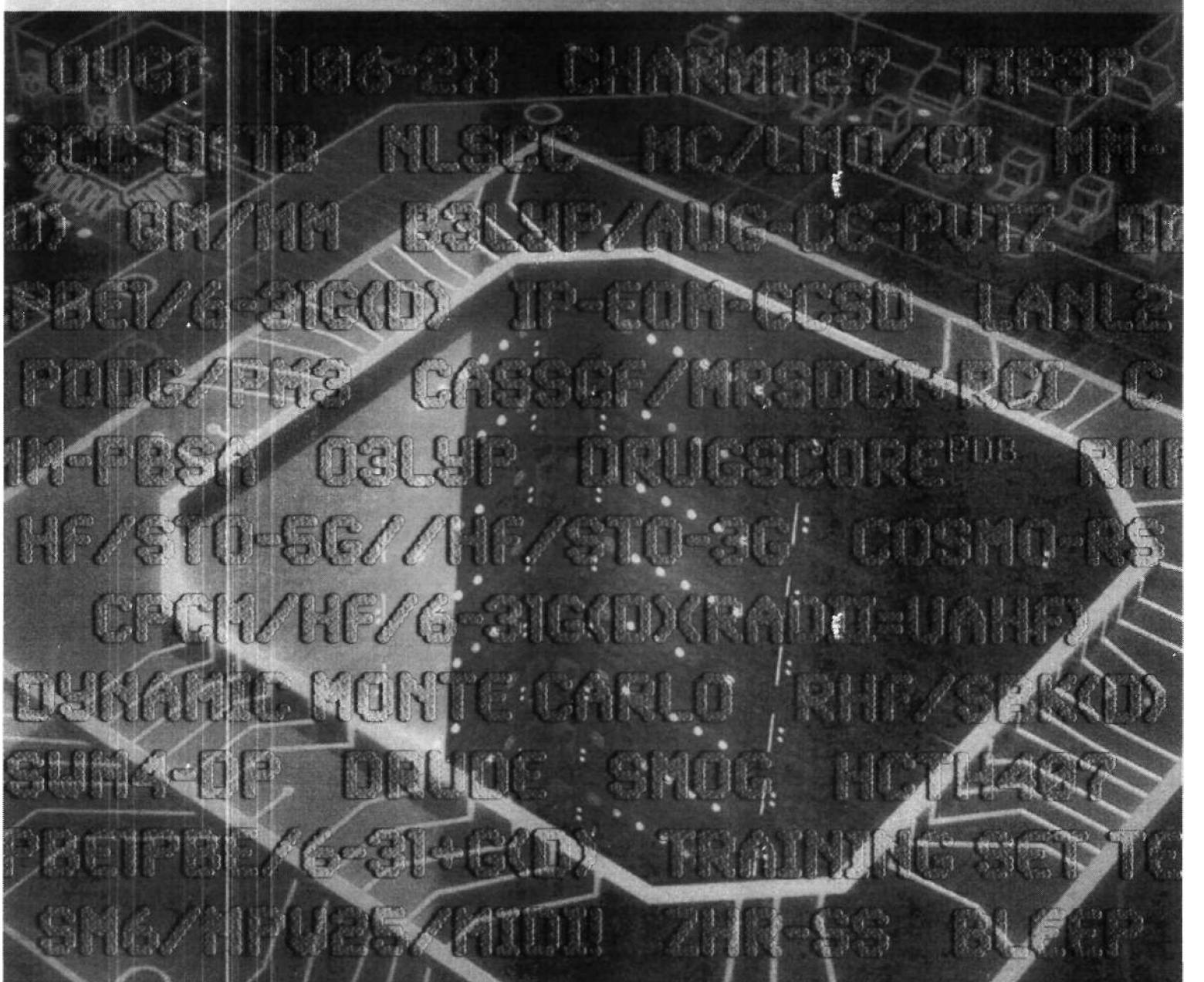

Springer

Calculation of melting points for binary ionic crystals of alkali metals halides

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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 $U_{i_a}t$ 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 [3J.

Subsequent transformation of the received expressions allowed to obtain the equation for *a priori* calculation of melting point of crystalline alkaline metals halides . This equation is based an the magnitudes of ionic radii , bond ionnity degree, masses and principal quantum numbers of elements, i.e. $T_{me}it = f(Ri , £l2 , m. , n,)$. The error of calculation of $T_{me}it$ makes -2,4%.

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).