



...the defect models have also shown that the properties that are retained character of the defect/abundance distribution are maintained in a data set, local crystal defect structure, etc.). The combination of both techniques enables the analysis of the distribution of the

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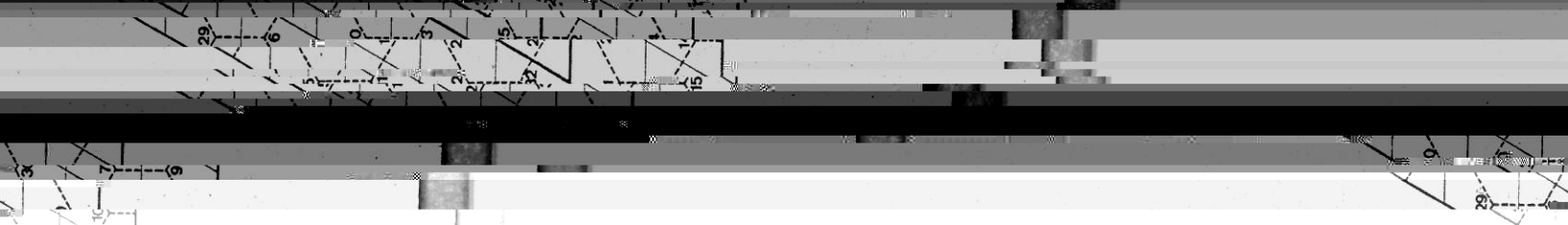
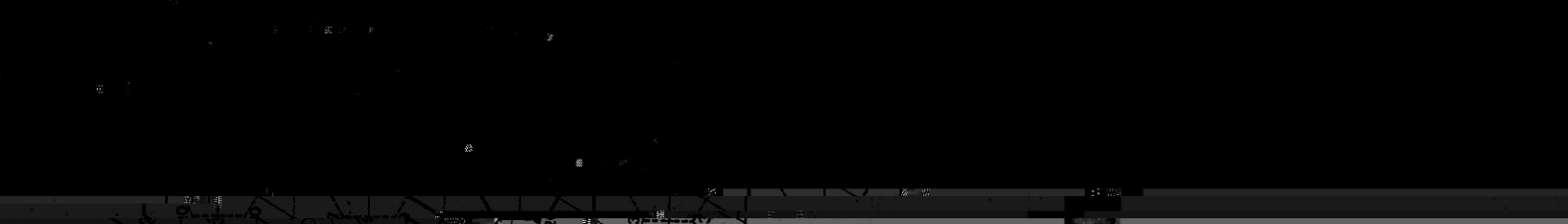
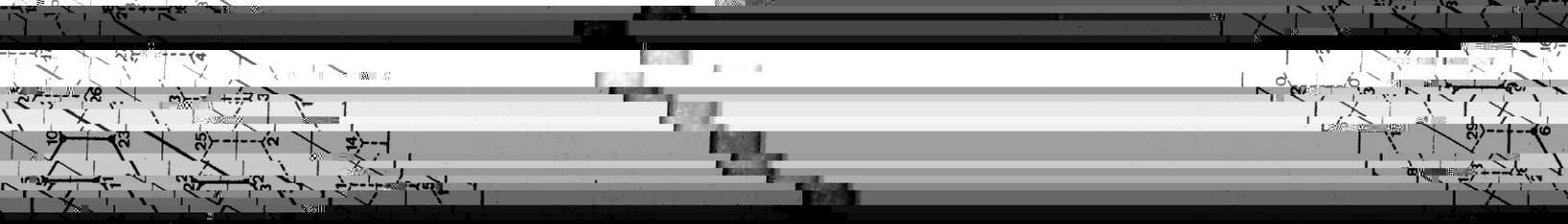
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with \mathbf{r} completely defined by $D(N_1)$, $D(N_2)$, $D(N_3)$ and $D(N_4)$, and with
the representation given in Eq. (1), for the calculation of the electronic energy
components to the calculation of the electronic energy of the molecule.



Fig. 1

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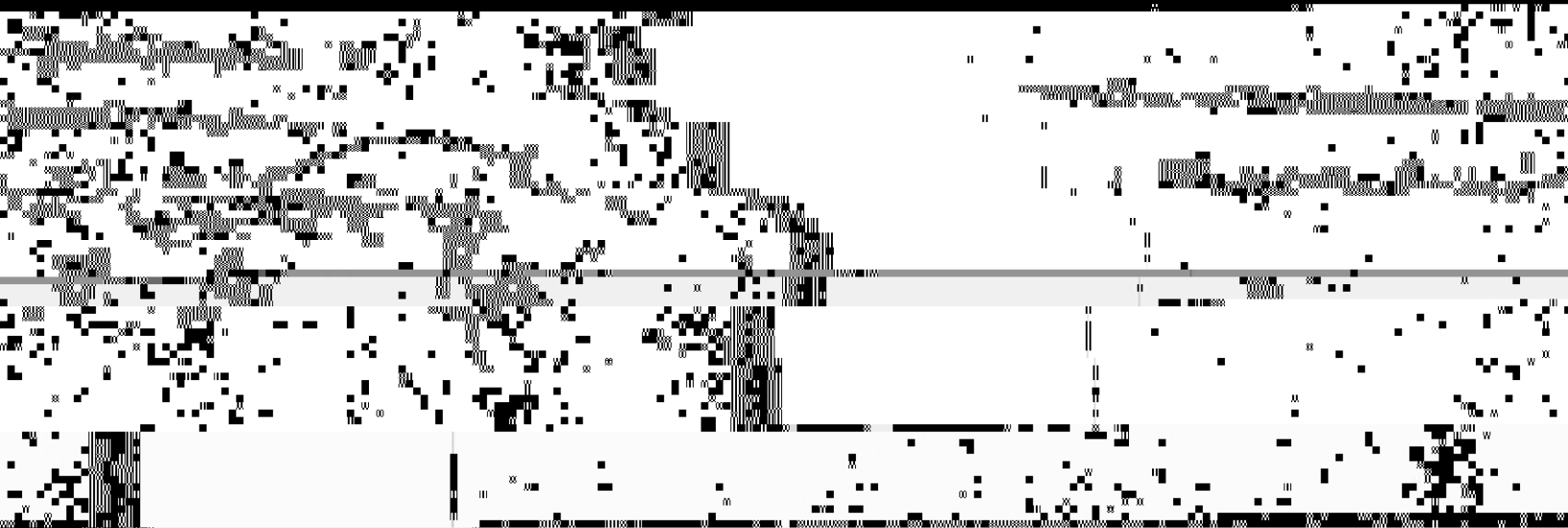


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... $2+2$ atoms ($N = 2$, a total
... 1111 ... even ...

... interaction range $n.a.$

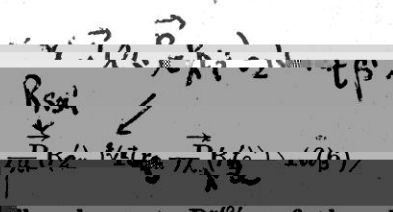
$S_{\alpha,\beta} = \langle \vec{r}_i - \vec{R}_\alpha | \hat{A} | \vec{r}_j - \vec{R}_\beta \rangle$



indirect interaction; it is independent on β

$$(\mu_{\alpha}, \lambda_{\beta} | \mu'_{\alpha'}, \lambda'_{\beta'}) =$$

$$= (1/\beta) \frac{\vec{R}_{\alpha} \cdot (\vec{R}_{\alpha} \times \vec{R}_{\beta})}{|\vec{R}_{\alpha}| |\vec{R}_{\beta}|} \frac{1}{|\beta|} \frac{\vec{R}'_{\alpha'} \cdot (\vec{R}'_{\alpha'} \times \vec{R}'_{\beta'})}{|\vec{R}'_{\alpha'}| |\vec{R}'_{\beta'}|} (\beta)$$



β is the angle between the elements μ and μ'

$$E_{\text{eff}} = \frac{1}{2} \sum_{\mu\nu, \lambda\sigma} \frac{P_{\mu\nu}^{\alpha\beta} P_{\lambda\sigma}^{\alpha\beta}}{P_{\mu\nu}^{\alpha\beta} P_{\lambda\sigma}^{\alpha\beta}} \sum_{\mu\nu, \lambda\sigma} \frac{Z_A Z_B}{R_{\mu\nu} R_{\lambda\sigma}} \quad (13)$$

and in the effective one-electron Hamiltonian, interpreted as

of a diatomic molecule, the chemical formula of a diatomic molecule in the ground state of the molecule is interpreted as the ground state of the molecule and the ground state of the molecule is interpreted as the ground state of the molecule.

used to calculate the elements in Eq. (3).

(b) Convergence of reciprocal space sums

problems (a) and (b) could be reduced to one if one

Conver

number of k_n

...representation, are uniquely determined.

...consistent with the matrix
in the orbital pair (see ...)

...in the non-spherical ...
...towards ...

$$\Delta E_{\text{tot}}(a) \approx A \Delta a^2 \quad (16)$$

Near the minimum, the first derivative method is ...

...isolated constituents. ...
...second derivative of $E_{\text{tot}}(a)$ with respect
to symmetrical ... is numerically evaluated ...

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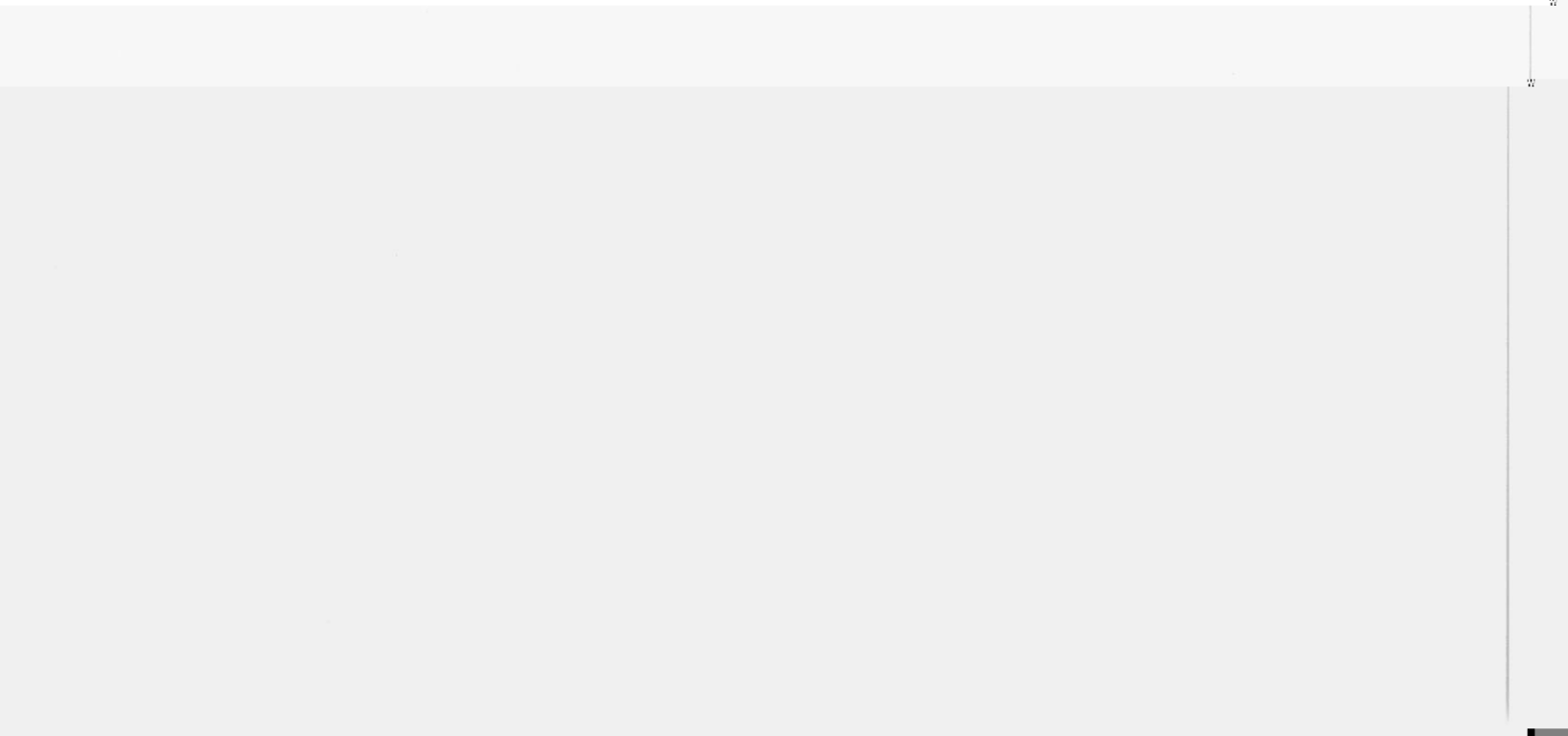
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consistent

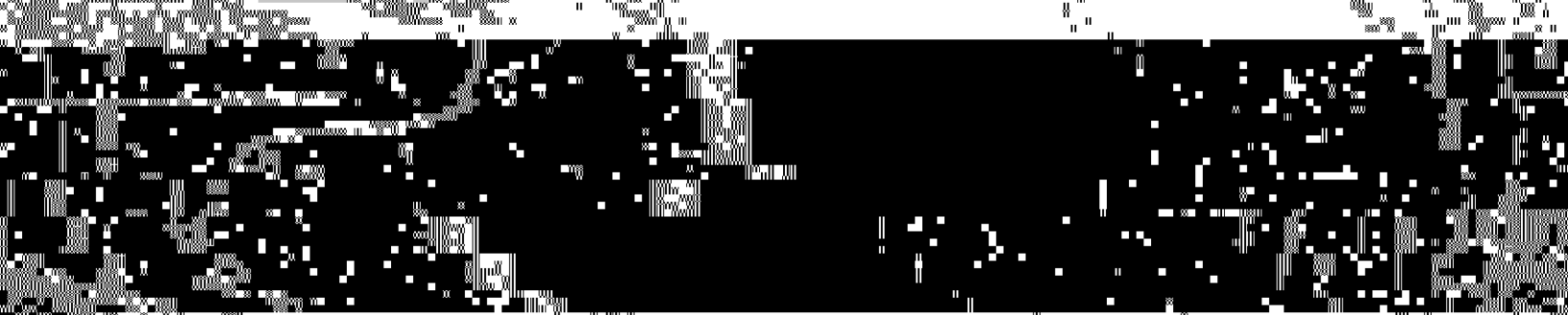
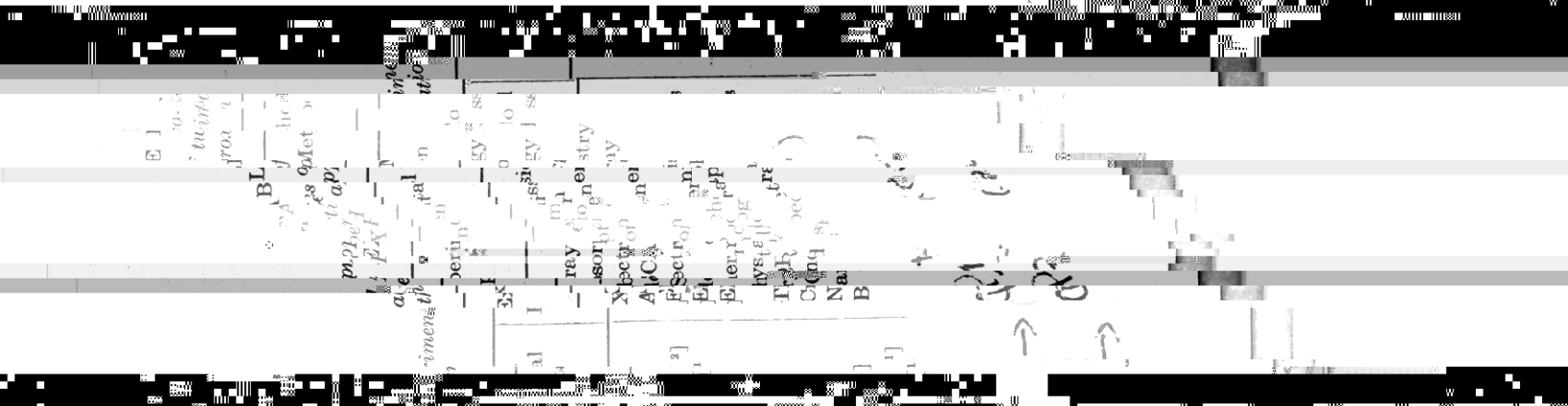
value of 1.1×10^4 is consistent with the experimental deter-

minally displaced

using the parameters $\mu_{22} = 21.4\%$, $\mu_{21} = 12.0\%$, $\mu_{11} = 12.0\%$ with $\mu_{12} = 12.0\%$ and $\mu_{20} = 12.0\%$. The observed agreement is consistent with most of the experimental data.

Next, the value of μ_{22} is determined by the following:

=



F^{avo}

0107.04b

P2000

8.0a d

(00) V1

2801.1 V1

Verdine

30.0d

(00) 1

34.5.6

P27.5.6

P27.5.6

27.5.6

27.5.6

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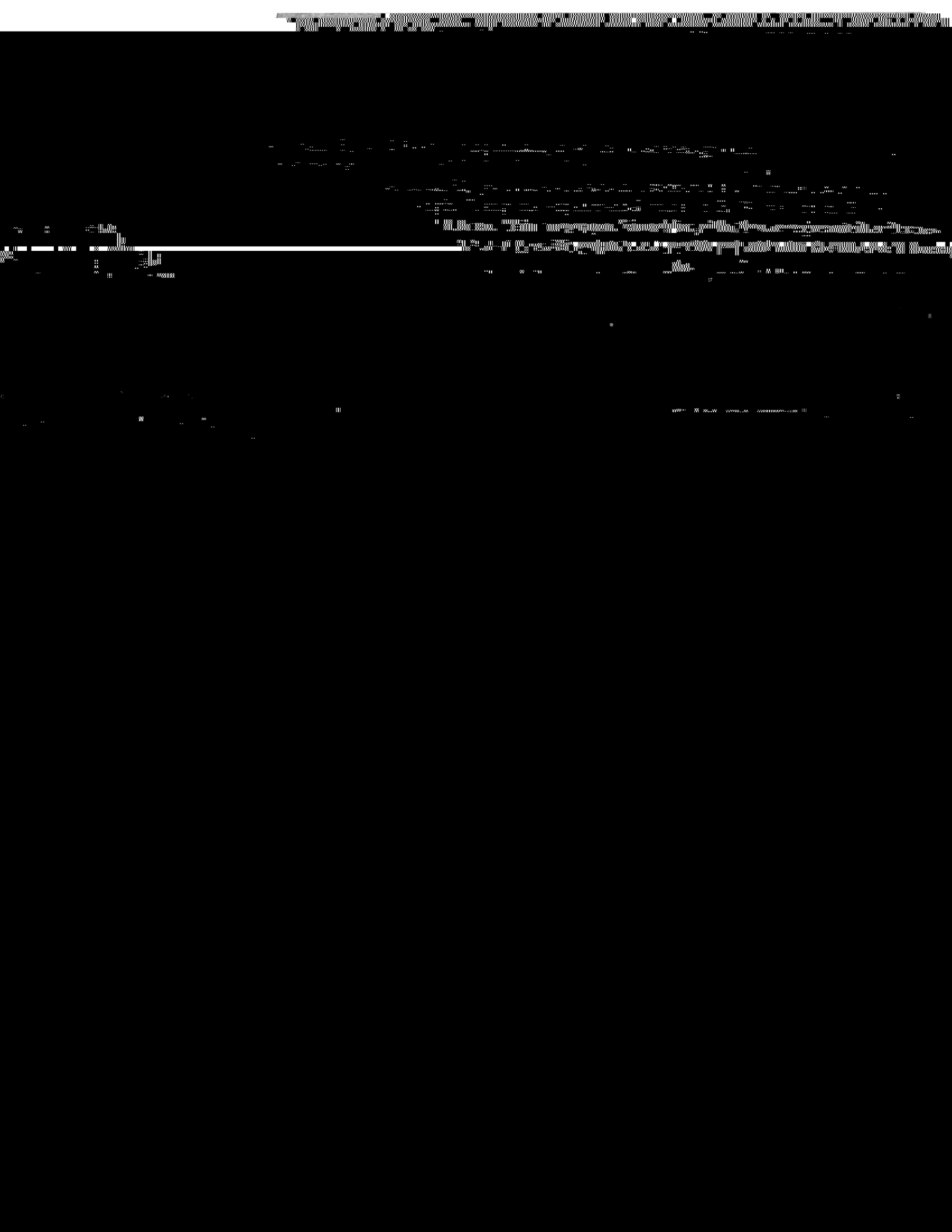
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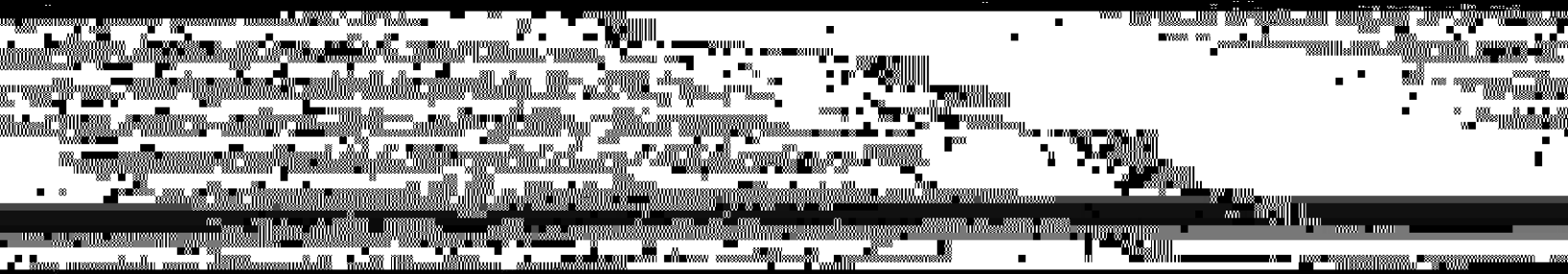
27.5.6



the crystal composition in the range of 2.73 Å to 2.49 Å

is shown in Figure 1. The crystal composition is given in Table I.

III



5000

d -R_{FF} = 2.73 Å

d -R_{FF} = 2.49 Å

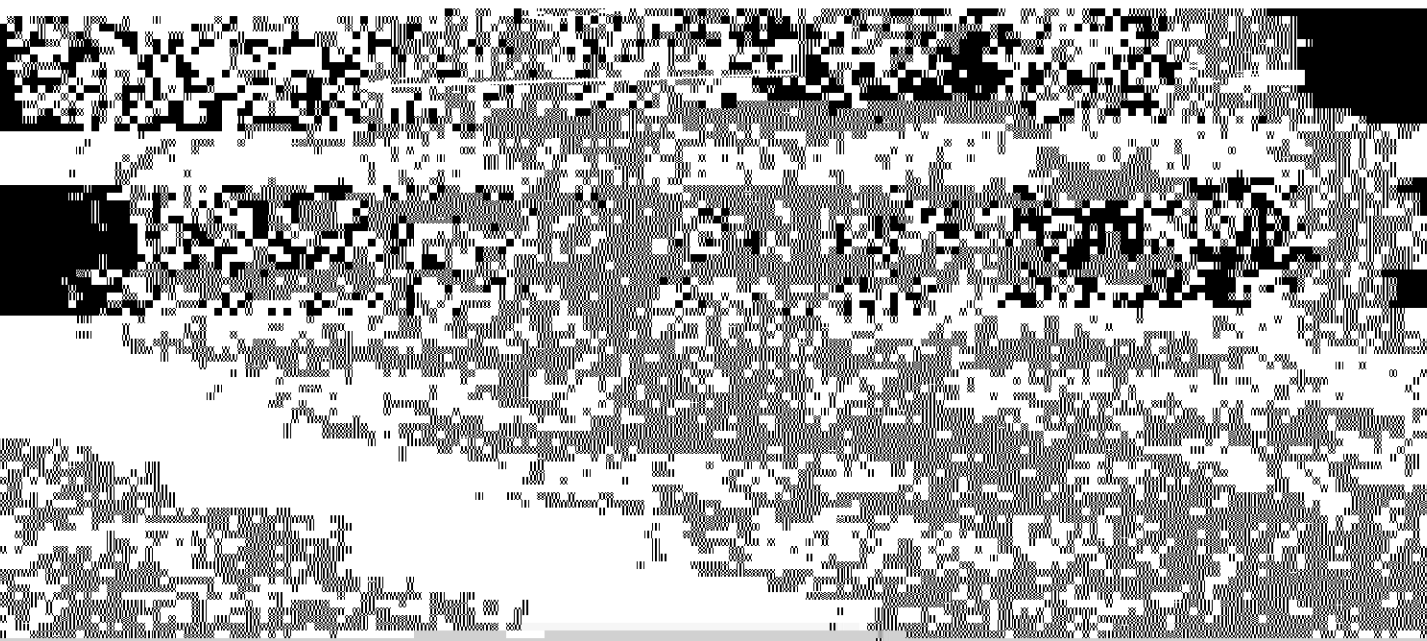
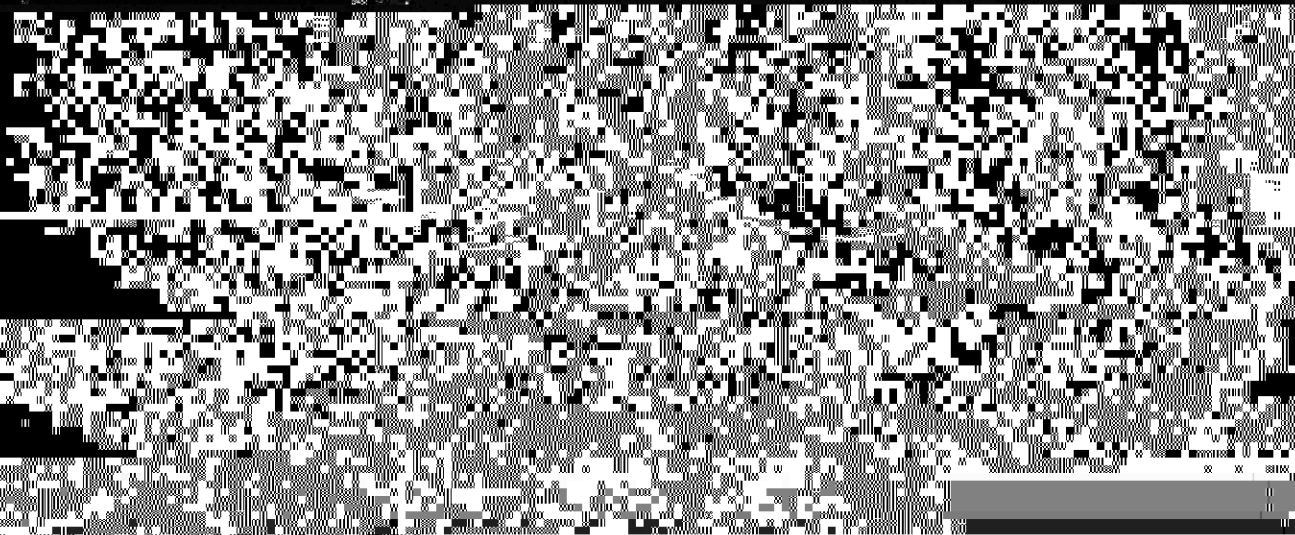
2.73 Å

Fig. 1. — Potentials for proton distribution in bond III.



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with recent experimental data [49]



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... 1963.

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... A. ZINBERG...

... R. HOFFM...

... HILL, N.Y., 1970.

... A. ZINBERG...

... Copyright ...

... 1963.

