II. THE SMALL-PERIODIC-CLUSTER (SPC) APPROACH

energy levels associated with point defects in the otherwise perfect

crystals bands at these N points can be calculated by solving the eigenvalue problem associated with an N-atom pseudomolecule

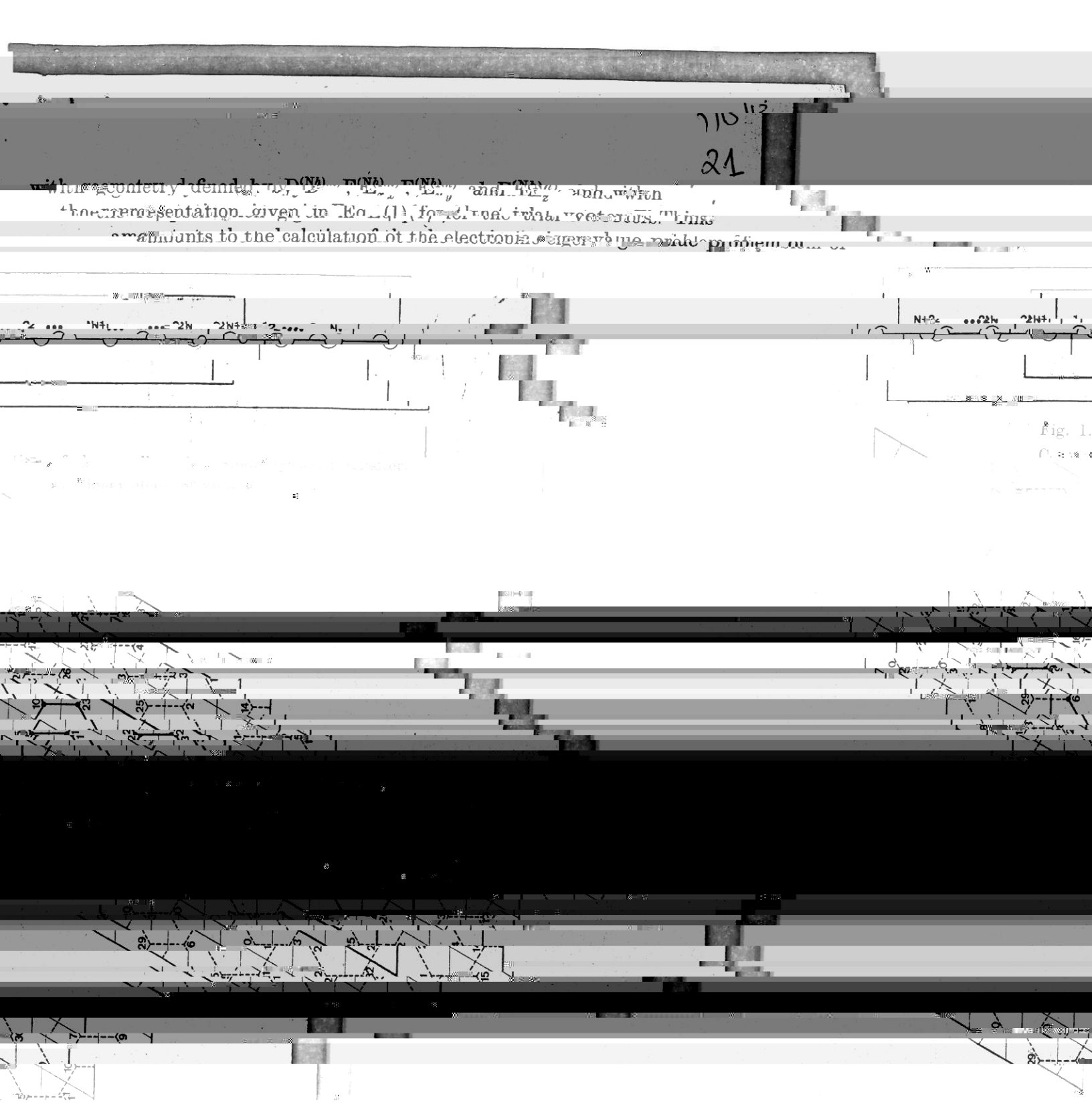


Fig. 1.

[redacted]

$$E_{tot} = \frac{1}{2} \sum_{\mu n, \lambda m, \alpha\beta} P^{\alpha,\beta}_{\mu n,\lambda m} \left[H^{\alpha,\beta}_{\mu n,\lambda m} + F^{\alpha,\beta}_{\mu n,\lambda m} \right] + \sum_{A<B} \frac{Z_A Z_B}{|R_A - R_B|} \tag{13}$$

and in the effective one-electron Hamiltonian matrix

[redacted]

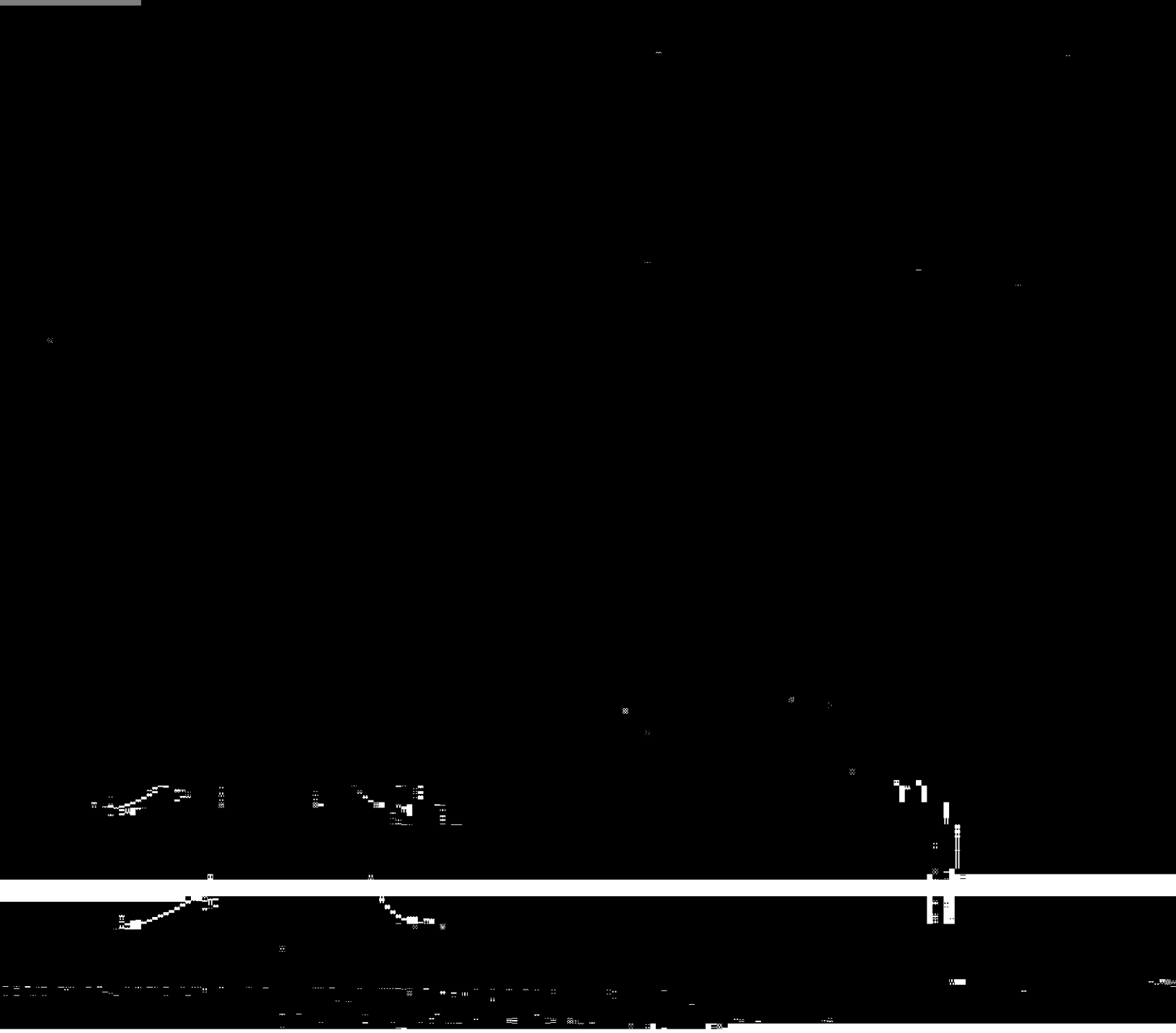
used to calculate the elements in Eq. (3).

(b) Convergence of reciprocal space summation

[redacted]

Conver

[redacted]




E_d
R.c-h
4.87eV.
e'_σ
a'_π
V.B.
a'_σ

consistent

[illegible]

X-ray [illegible]
Absorption [illegible]
X[illegible] Spectr[illegible]
A[illegible] ESCA
[illegible] Spectr[illegible]
El[illegible]
Energy [illegible]
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T[illegible]
C[illegible]
N[illegible]
B[illegible]

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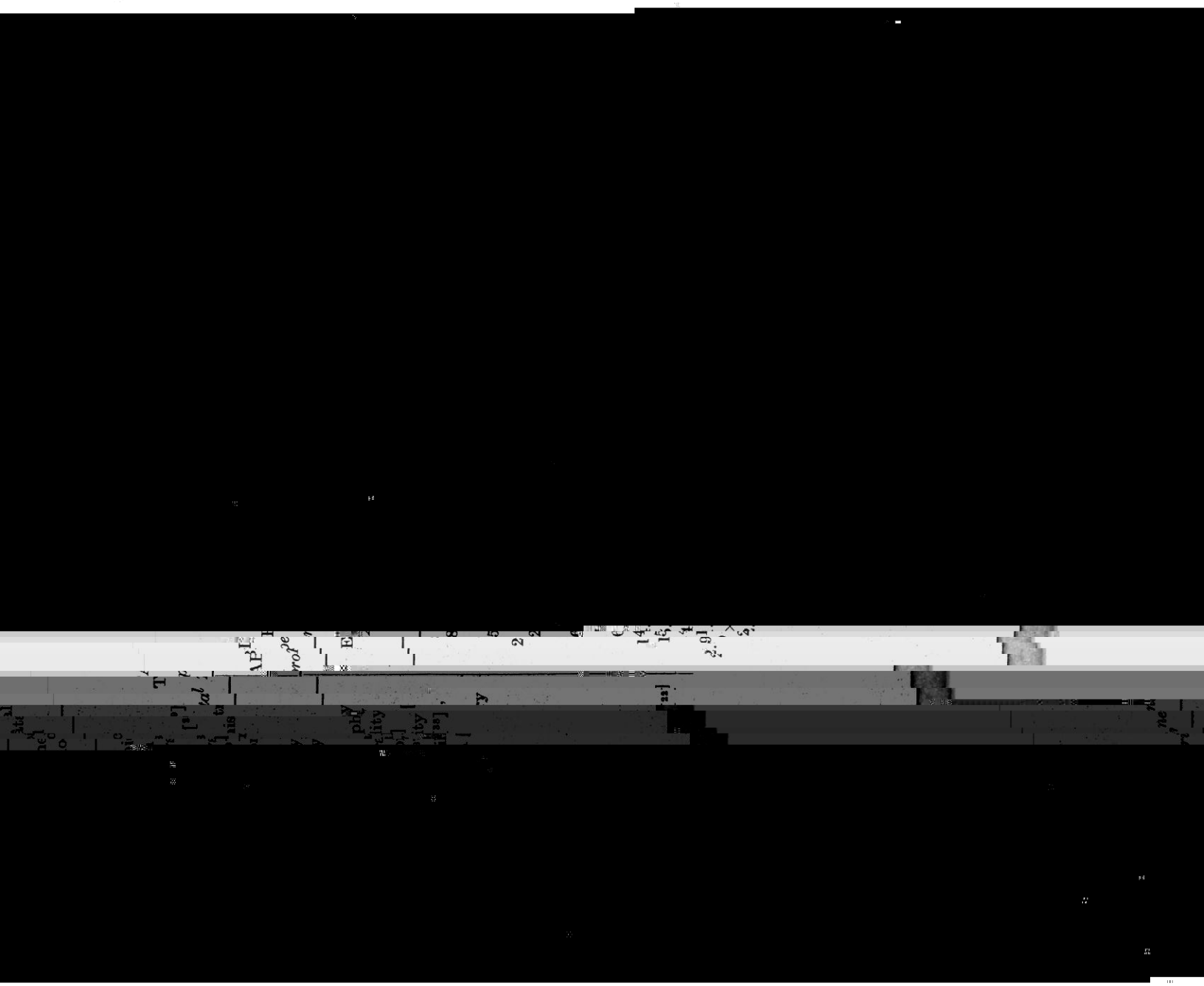


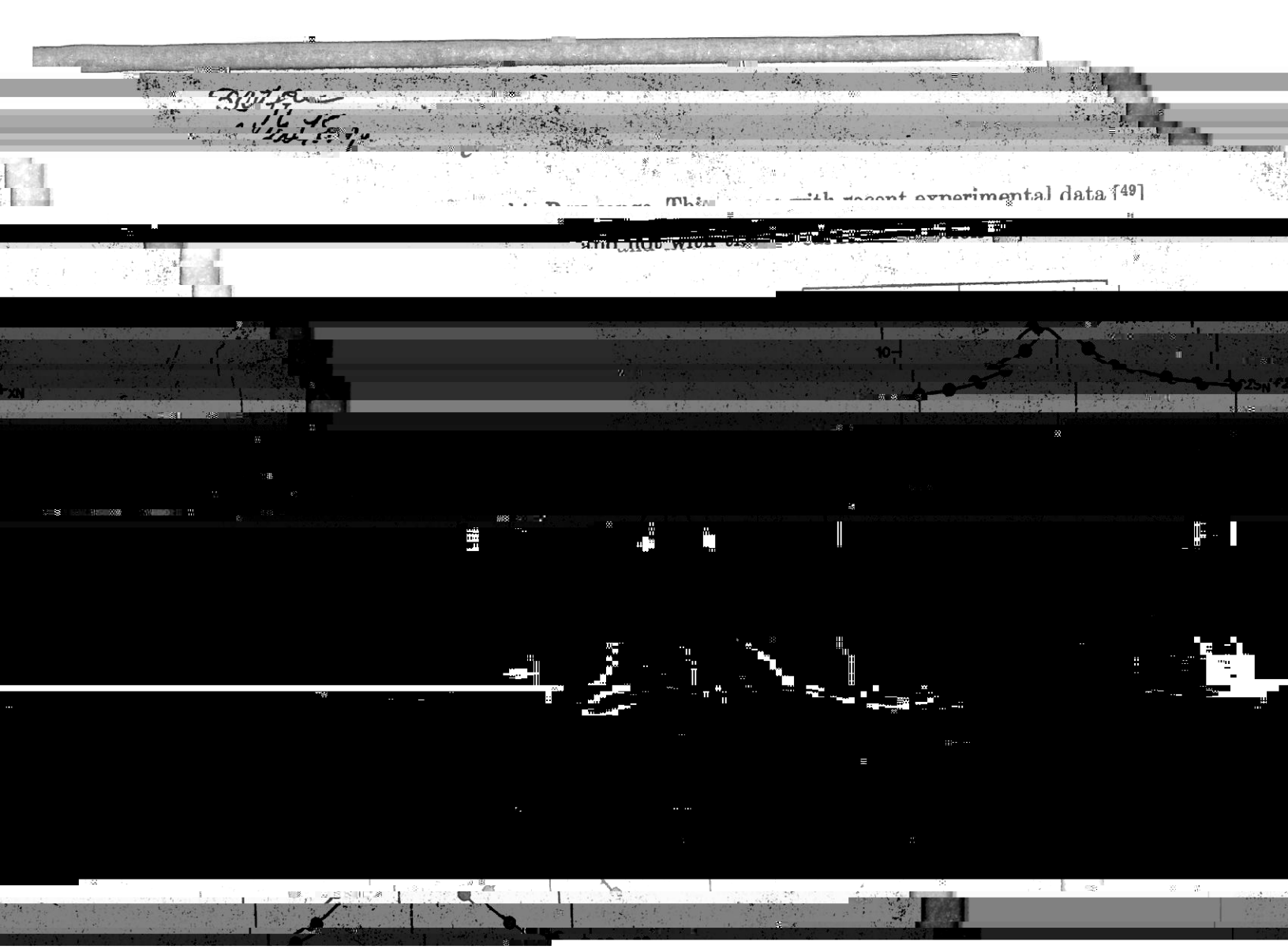
[redacted]


$R_{FF} = 2.73Å$
$R_{FF} = 2.49Å$

required to form an ionic Bjerrum defect (by translating a proton to the opposite end of the potential well) is calculated to be 83.9 kcal/mole.

populated band is only half occupied in the ground state resulting

with recent experimental data [49]



Hill, N.Y.), 1970.