

# The Fluorine Distribution in Cristobalite Substituted with Boron

Composition of  $\text{B}_2\text{O}_3$  10-20 mol.-%

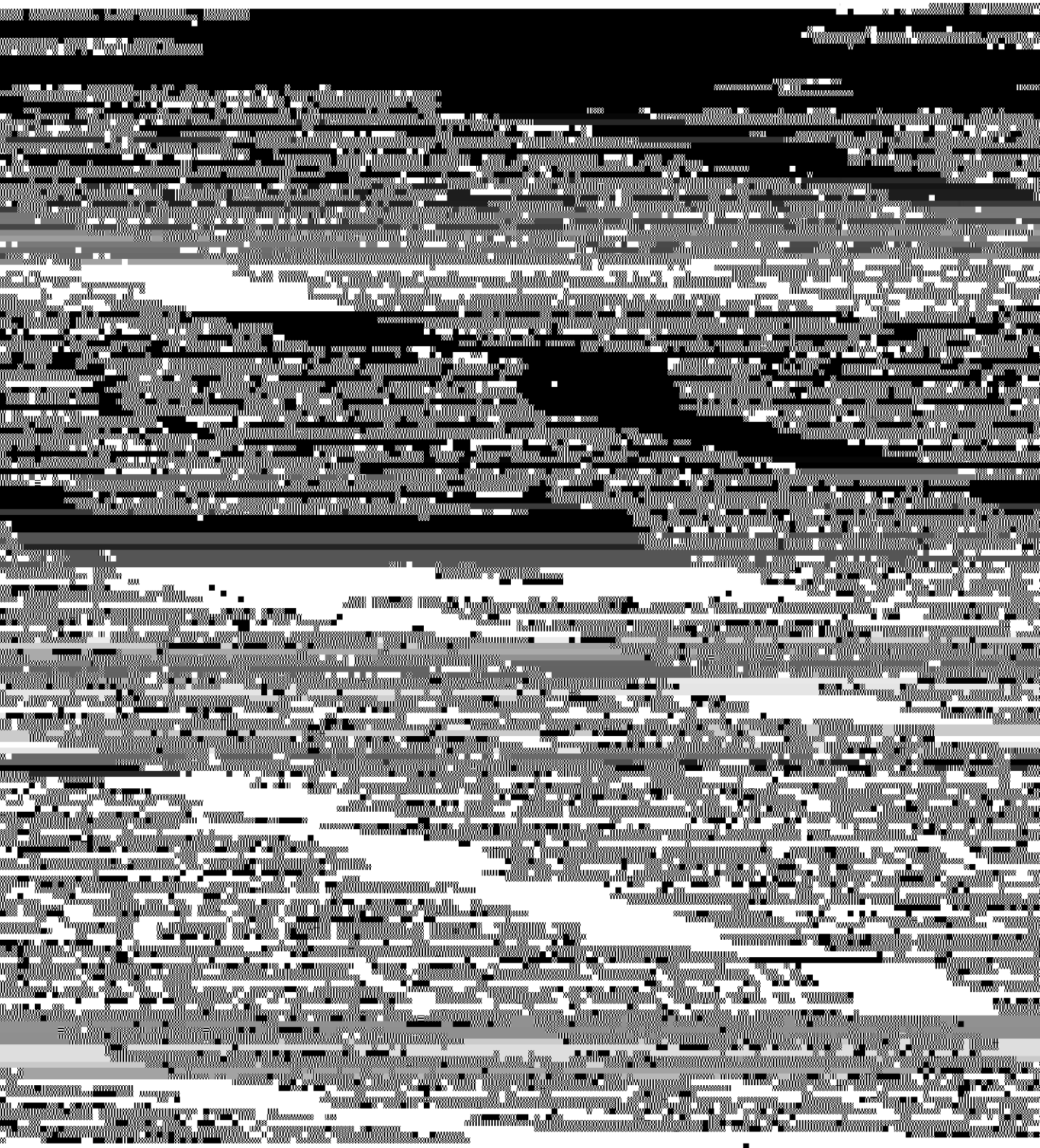


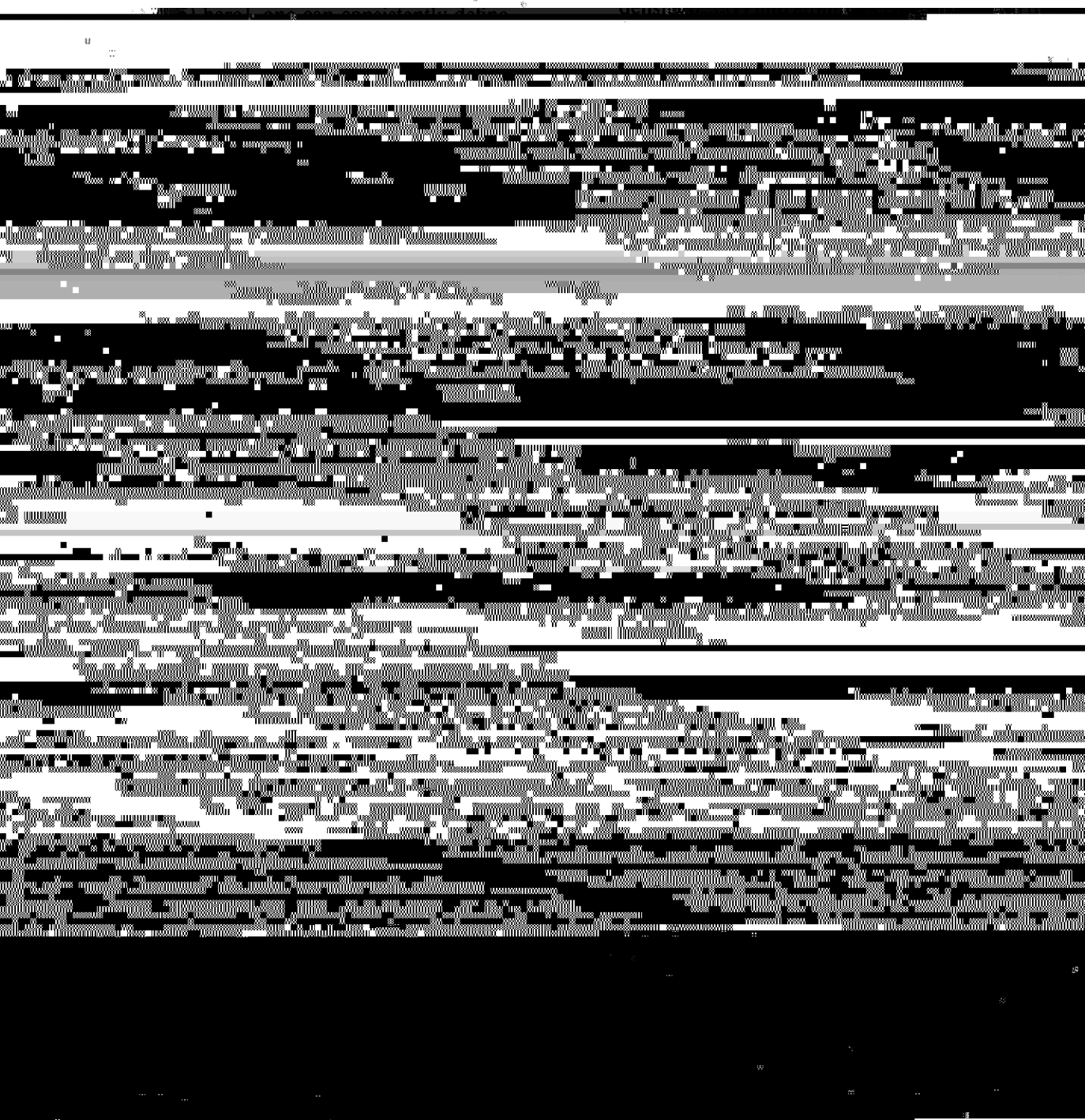
Table I. Dynamic  $\rho(\mathbf{r}, \omega)$  and static  $\rho(\mathbf{r}, 0)$  structure factors for Si, in units of  $e/a^3$

The experimental data are corrected for anomalous dispersion and nuclear scattering. In parentheses the estimated standard deviations are given

$\omega$	$\rho(\mathbf{r}, \omega)$	$\rho(\mathbf{r}, 0)$	$\rho(\mathbf{r}, \omega)$	$\rho(\mathbf{r}, 0)$	$\rho(\mathbf{r}, \omega)$	$\rho(\mathbf{r}, 0)$	$\rho(\mathbf{r}, \omega)$	$\rho(\mathbf{r}, 0)$	$\rho(\mathbf{r}, \omega)$	$\rho(\mathbf{r}, 0)$
220	8.397	8.3881	2.9	-3	10.455	-1.48	10.720	10.720	10.720	10.720
331	7.694	7.6834	1.9	1.83	7.814	-1.33	8.065	8.065	8.065	8.065
444	0.161	0.1620	0.0	0.0	0.000	-0.17	0.168	0.168	0.168	0.168
555	4.444	4.444	1.0	1.0	4.107	-0.33	4.468	4.468	4.468	4.468
666	3.931	3.931	0.0	0.0	3.931	0.0	3.931	3.931	3.931	3.931

the total charge density  $\rho(\mathbf{r}, \omega)$  is given as a convolution of the static charge density  $\rho(\mathbf{r}, 0)$  and the dynamic smearing function  $\rho(\mathbf{r}, \omega)$ . (i) Core and valence wavefunctions are  $\psi_c(\mathbf{r})$  and  $\psi_v(\mathbf{r})$  respectively. (ii) As a first approximation, the total charge density is given by  $\rho(\mathbf{r}, 0) = \sum_i Z_i \delta(\mathbf{r} - \mathbf{r}_i)$ , where  $\mathbf{r}_i$  is the position vector of an ion of charge  $Z_i$  at position  $\mathbf{r}_i$ . The total charge density is given by  $\rho(\mathbf{r}, 0) = \sum_i Z_i \delta(\mathbf{r} - \mathbf{r}_i) + \rho(\mathbf{r}, 0)$ , where  $\rho(\mathbf{r}, 0)$  is the static charge density.

[The following table content is heavily corrupted and illegible due to severe image noise. It appears to be a large table with multiple columns and rows, possibly representing a joint density function structure as mentioned in the caption.]





formation...  
minimally...  
Fig. 1(b). In contrast, the corresponding density  $\rho_{\text{eff}}(\mathbf{r})$  has minimum...  
Fig. 2

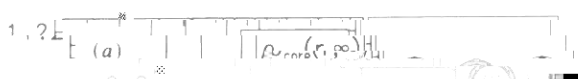


Fig. 1(b). In contrast, the corresponding density  $\rho_{\text{eff}}(\mathbf{r})$  has minimum...

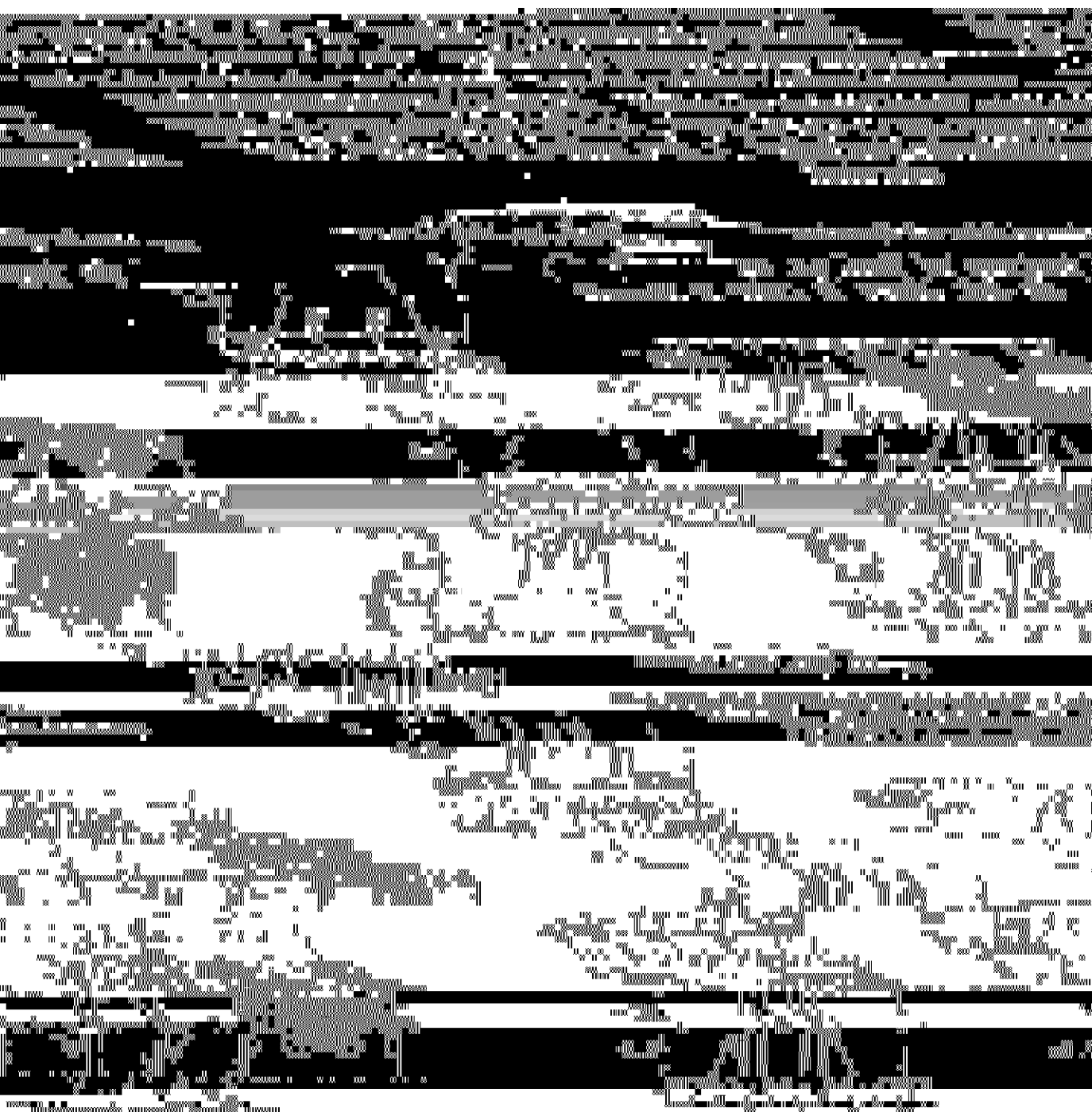


the same...  
= 0.1...  
Fig. 2...  
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The latter...

As (5.20) of Fig. 2(c) (except for the inner core) included in the Fourier series  $\hat{u}_\epsilon$  to model the behavior at low  $\epsilon$ . In Fig. 4, clearly, the behavior of  $\hat{u}_\epsilon$  near the outer boundary is nearly independent of  $\epsilon$ . In Fig. 4, clearly, the behavior of  $\hat{u}_\epsilon$  near the outer boundary is nearly independent of  $\epsilon$ . In Fig. 4, clearly, the behavior of  $\hat{u}_\epsilon$  near the outer boundary is nearly independent of  $\epsilon$ .



Fig. 6. The charge distribution calculated for  $Q = 0.55$  e. The contour peaks differ from Debye's model (contour  $Q = 0.5$  e).



The contours are labeled with numerical values representing the charge density. The plots show the charge distribution for different values of Q, with the top plot for Q = 0.55 e and the bottom plot for Q = 0.5 e. The contours are labeled with values such as 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9, 4.0, 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 5.0, 5.1, 5.2, 5.3, 5.4, 5.5, 5.6, 5.7, 5.8, 5.9, 6.0, 6.1, 6.2, 6.3, 6.4, 6.5, 6.6, 6.7, 6.8, 6.9, 7.0, 7.1, 7.2, 7.3, 7.4, 7.5, 7.6, 7.7, 7.8, 7.9, 8.0, 8.1, 8.2, 8.3, 8.4, 8.5, 8.6, 8.7, 8.8, 8.9, 9.0, 9.1, 9.2, 9.3, 9.4, 9.5, 9.6, 9.7, 9.8, 9.9, 10.0.





1987, 1987, 1987

the multipole moments are calculated in the  
of simple radial functions

RE, R. W., VAN, W. R., & SCHUBERT  
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