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...esame Equation of State Number 7411, Al_2O_3

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LA-11058-MS

UC-34
Issued: August 1987

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J. F. Barnes
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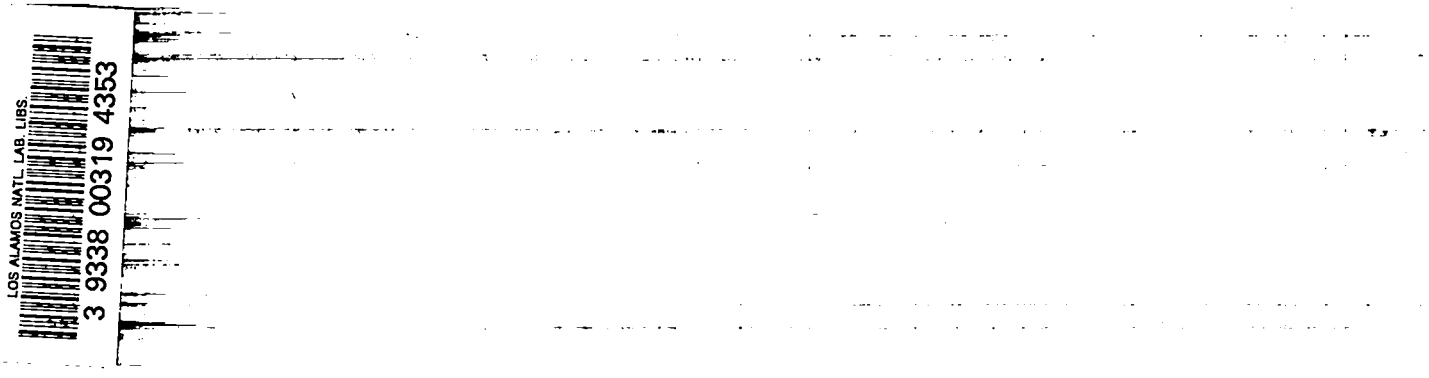

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SESAME EQUATION OF STATE NUMBER 7411, $A\ell_2O_3$

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and
S. P. Lyon

ABSTRACT

A new global equation of state for $A\ell_2O_3$ ("alumina") has been constructed and placed on the SESAME Library as material number 7411.

The compound $A\ell_2O_3$, "alumina", occurs abundantly in nature as the mineral corundum. A SESAME equation of state (EOS), material number 7410, was created for alumina in 1972. However, some of the physics models used in producing global EOSs for the data library have changed considerably since that time; in particular, J. D. Johnson's improved treatment[1] (CHART JD Model) of the ion thermal (nuclear) contribution to pressure and energy has been incorporated into the GRIZZLY[2] code and is used as the preferred model. Because of the importance of corundum to mixture EOSs for various soils, we considered it advisable to produce a revised global EOS for the material, and it has been placed on the library as EOS number 7411. Although it turned out that there is no apparent large difference between 7410 and 7411, we do recommend usage of the newer EOS.

Alumina exhibits a very high shear strength which has a considerable effect on the experimentally obtained shock Hugoniot. The data are

thoroughly discussed by Graham and Brooks[3]. The shear offset must be corrected for in constructing an equilibrium equation of state; here we accomplish this by simply representing the U_s-U_p shock data as given in Marsh[4] by a single straight line through the high pressure data with an intercept at the experimentally obtained bulk sound speed. We used the fit $U_s = 7.93 + 1.298\ U_p$ km/s. Shock data were matched to the Thomas-Fermi Dirac calculations at a compression of 1.35.

We used the GRIZZLY code and treated the compound as an average atom with atomic number $\bar{Z} = 10.0$ and atomic weight $\bar{A} = 20.392$. Density at room temperature was taken as 3.97 g/cm^3. GRIZZLY constructed the cold curve using the default formulation of the Grüneisen parameter

$$\gamma(\eta) = \gamma_o \left(\frac{1}{\eta}\right) + \frac{2}{3} \left[1-\left(\frac{1}{\eta}\right)\right]^2$$

with $\gamma_o = 1.595$, which is both the thermodynamic value and the 2S+1 value from the shock data. The Debye, or characteristic, temperature was calculated to be 1034 K from longitudinal and transverse sound speeds.

The cohesive energy, or energy required to separate $A\ell_2O_3$ into 5 separate atoms at 0 K, was calculated as 725 kcal/mole, or 145 kcal/mole for the average atom. The form of the cold curve in expansion was then adjusted with the Lennard-Jones (L-J) parameter in an attempt to produce a critical temperature close to our very rough estimate of 1 eV, a figure based on the known boiling point of $A\ell_2O_3$. It proved not to be possible to lower the calculated T_c beneath about 14,600 K without severely disturbing the calculated isotherms. The corresponding value of the L-J parameter is 0.5.

The following graphs were made for EOS 7411 using the SES2D graphics code. Figures 1 and 2 are the pressure and energy isotherms plotted over the entire temperature range of the tables. Figure 3 shows shock speed versus particle speed along the principal Hugoniot, as used in the model.

REFERENCES

1. J. D. Johnson, private communication.

2. J. Abdallah, Jr., "User's Manual for GRIZZLY," Los Alamos National Laboratory report LA-10244-M (September, 1984).

3. R. A. Graham and W. P. Brooks, J. Phys. Chem. Solids 32, 2311 (1971).

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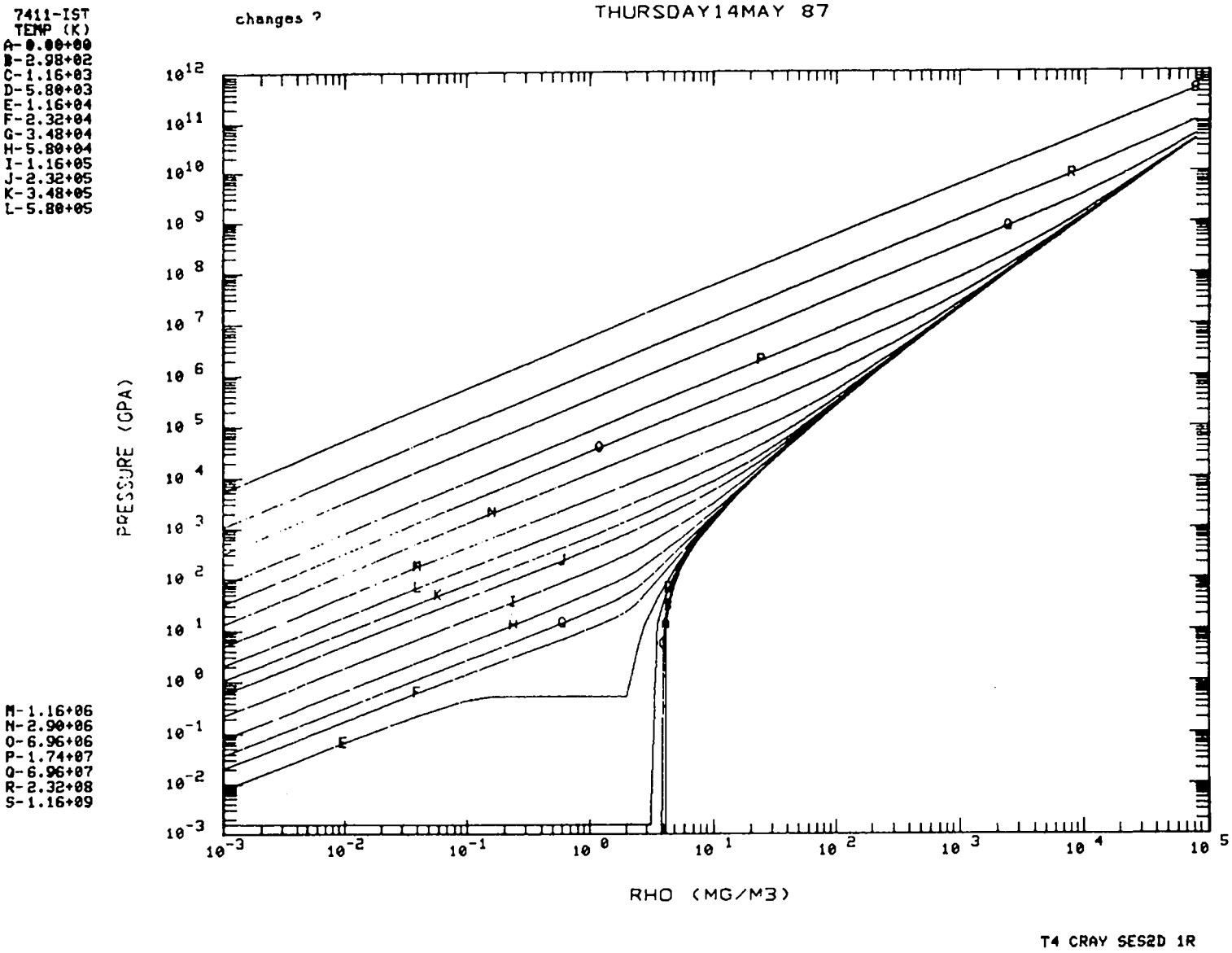

Figure 1. Selected pressure isotherms for EOS 7411

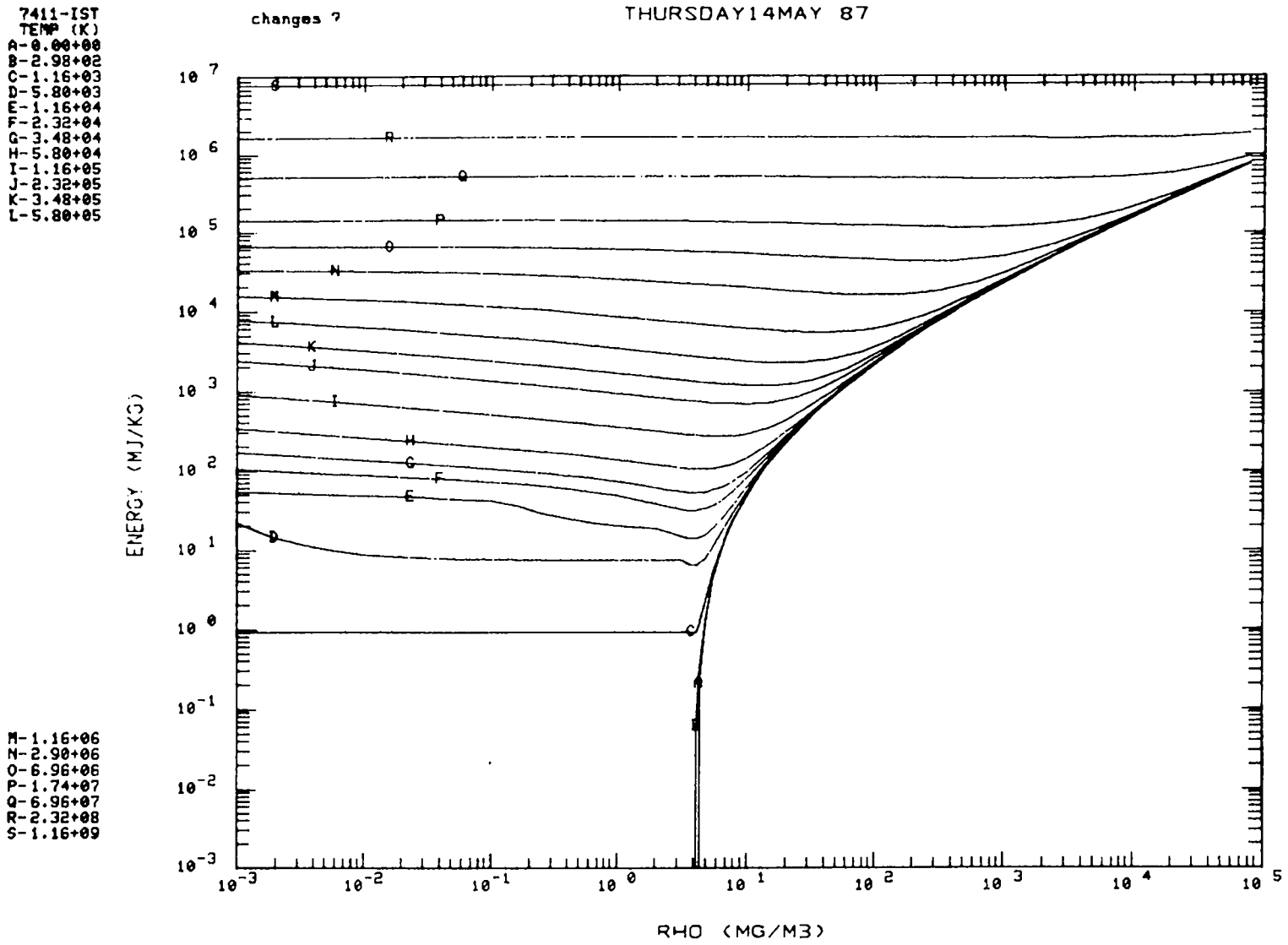

Figure 2. Selected energy isotherms for EOS 7411

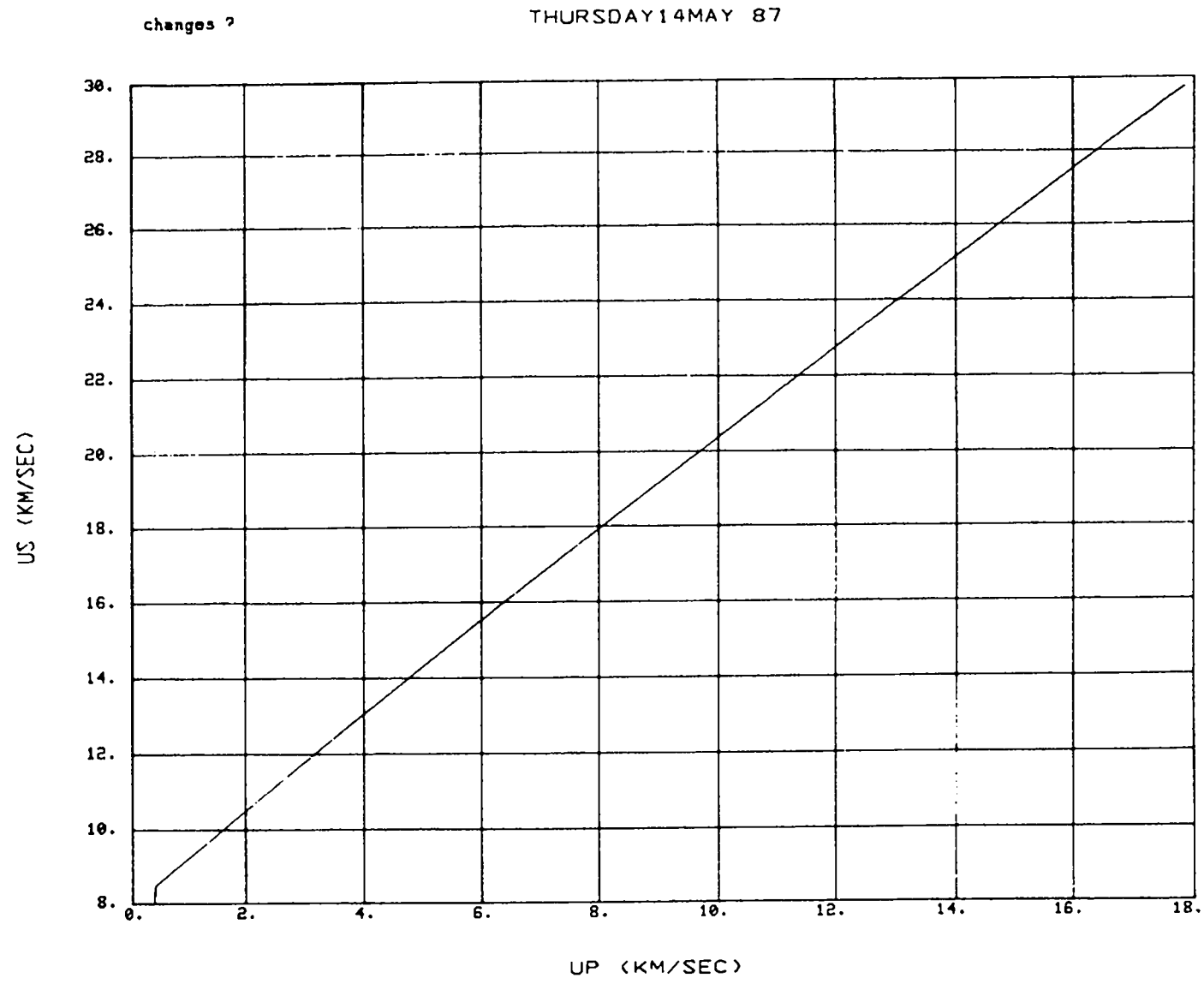

Figure 3. Shock velocity versus particle velocity along the principal Hugoniot for EOS 7411

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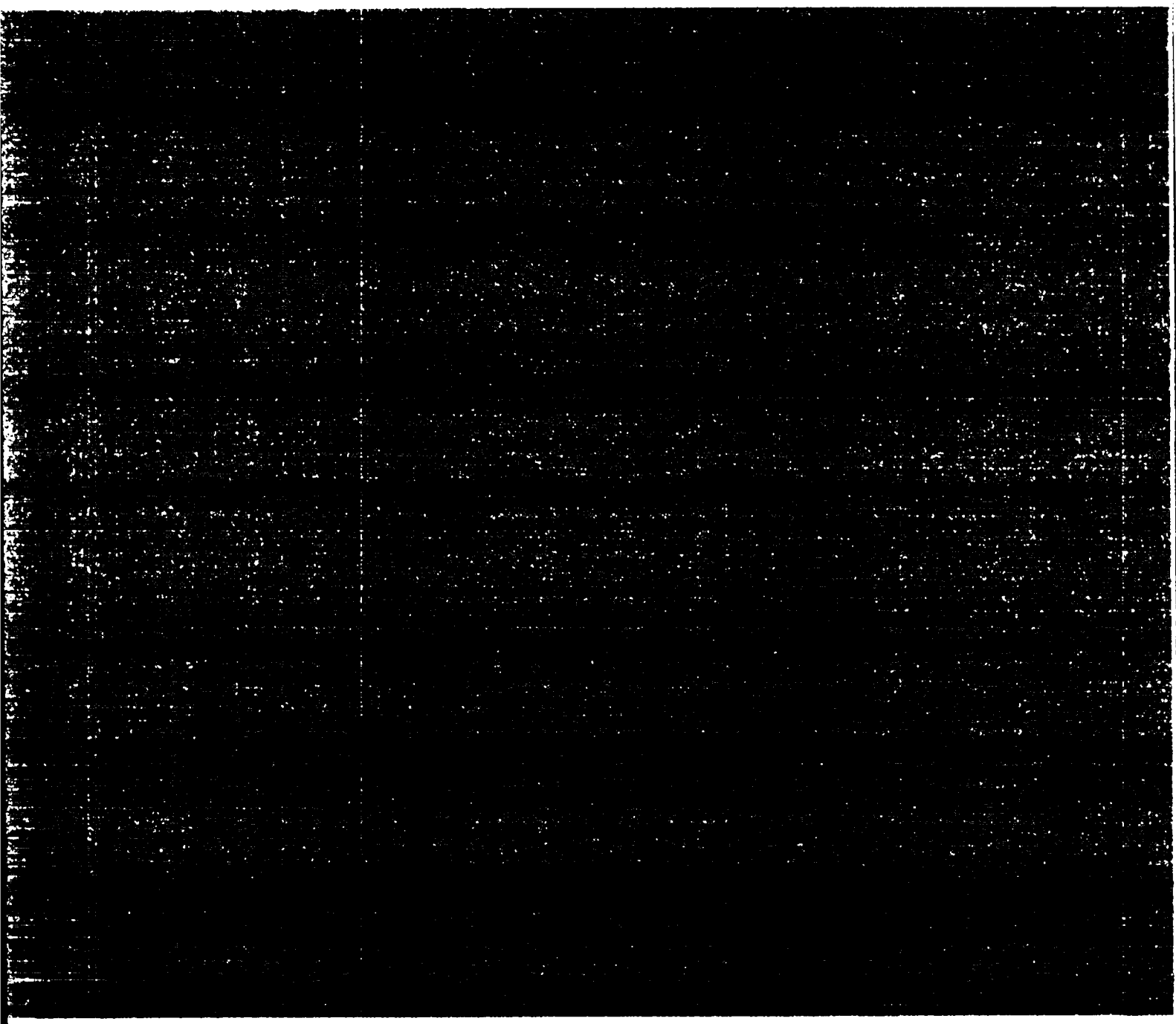

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