**PACKAGE ID -** 001050SUN0000 EDEN

**KWIC TITLE -** Holographic Methods in X-ray Crystallography

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**LIMITATION CODE -**UNL **AUDIENCE CODE -** UNL

**COMPLETION DATE -** 04/21/1993 **PUBLICATION DATE -** 04/01/1993

**DESCRIPTION -** The holographic method makes use of partially modeled electron density and experimentally-measured structure factor amplitudes to recover electron density corresponding to the unmodeled part of a crystal structure. This paper describes a fast algorithm that makes it possible to apply the holographic method to sizable crystallographic problems. The algorithm uses positivity constraints on the electron density, and can incorporate a target electron density, making it similar to solvent flattening. Using both synthetic and experimental data, we assess the potential for applying the holographic method to macromolecular x-ray crystallography.

**PACKAGE CONTENTS -** Media Directory; Software Abstract; READ.ME File (9 pages); Media Includes Source Code, Compilation Instructions, Sample Problem Input and Output, Programmer Documentation;

**SOURCE CODE INCLUDED? -** Yes

**MEDIA QUANTITY -** 1 CD Rom

**COMPUTER -** SUN

**OPERATING SYSTEMS -** UNIX

**PROGRAMMING LANGUAGES -** FORTRAN

**SOFTWARE LIMITATIONS -** There are about 30 input parameters, including: unit cell parameters (a,b,c angles and symmetry group); file information (names of .fobs and .fcalc files, as well as names of files containing physical space models, targets, weights and masks); and computational parameters (grid spacing, data resolution for reading data0.

**SOURCE CODE AVAILABLE (Y/N) -** Y

**RELATED SOFTWARE -** ADD, APODIZE, BACK, DPHASE, DRHO, FORTH, REGRID.

**REFERENCES -** J.R. Somoza, H. Szoke, D.M. Goodman, P. Beran, D. Trucks, S. Kim and A. Szoke, Holographic Methods in X-ray Crystallography IV., April 1993.

**ABSTRACT STATUS -** Submitted July 17, 1995. Released screened 7/28/95.

**SUBJECT CLASS CODE -** W

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**KEYWORDS -**
COMPUTER PROGRAM DOCUMENTATION
E CODES
HOLOGRAPHY
X-RAY DIFFRACTION

**EDB SUBJECT CATEGORIES -**
990200 665100 440800

**SPONSOR -** DOE/DP

**PACKAGE TYPE -** SCREENED