

**PACKAGE ID** - 000753IBMPC00 SHAPES

**KWIC TITLE** - Algorithm for Finding Similar Shapes in Large  
Molecular Structures Libraries

**AUTHORS** - Hagstrom, R.  
Argonne National Lab., IL (United States)  
  
Young, R.  
Argonne National Lab., IL (United States)

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

**COMPLETION DATE** - 09/01/1992   **PUBLICATION DATE** - 01/01/1993

**DESCRIPTION** - The SHAPES software consists of methods and algorithms for representing and rapidly comparing molecular shapes. Molecular shapes algorithms are a class of algorithm derived and applied for recognizing when two three-dimensional shapes share common features. They proceed from the notion that the shapes to be compared are regions in three-dimensional space. The algorithms allow recognition of when localized subregions from two or more different shapes could never be superimposed by any rigid-body motion. Rigid-body motions are arbitrary combinations of translations and rotations.

**PACKAGE CONTENTS** - Media Directory; Software Abstract; User's Manual;  
Media Includes Source Code;

**SOURCE CODE INCLUDED?** - Yes

**MEDIA QUANTITY** - 1 3.5 Diskette

**METHOD OF SOLUTION** - These algorithms succeed without ever performing rotations; instead, they characterize a large variety of different localized subregion shapes by: a. analytically representing some region as a sum of Gaussian functions; b. analytically representing the subregions each as sums of Gaussian functions; c. analytically expanding and then truncating representations of the subregions in terms of an orthonormal basis of radial associated Laguerre polynomials, altitudinal associated Legendre functions, and azimuthal exponential functions; d. computing a finite list of quadratic rotation-invariant scalars from the surviving expansion coefficients.

**COMPUTER** - IBM PC

**OPERATING SYSTEMS** - DOS

**PROGRAMMING LANGUAGES** - FORTRAN

**SOFTWARE LIMITATIONS** - NATOMS < 10,000.

**PACKAGE ID** - 000753IBMPC00 SHAPES

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

**TIME REQUIREMENTS** - The time required is linear in NATOMS.  
Approximately 10 seconds are needed when the value of NATOMS =  
1000.

**REFERENCES** - Ray Hagstrom and Richard Young, Algorithm for Rapidly  
Recognizing Shape Similarities among Large Libraries of Molecular  
Structures, 1993.

**ABSTRACT STATUS** - Released AS-IS 5/12/95.

**SUBJECT CLASS CODE** - WY

**KEYWORDS** -

COMPUTER PROGRAM DOCUMENTATION  
S CODES  
MOLECULAR STRUCTURE  
ROTATION  
THREE-DIMENSIONAL CALCULATIONS  
PATTERN RECOGNITION  
LIBRARIES  
SHAPES  
PROPER MOTION

**EDB SUBJECT CATEGORIES** -  
990200 664000 661100

**SPONSOR** - DOE/EH

**PACKAGE TYPE** - AS - IS