

PACKAGE ID - 000265D078000 VIVAS2

KWIC TITLE - A-BC Exact Coupled Channel Scattering

AUTHORS - Parker, G.A.
University of Oklahoma, Norman, OK (United States)

Light, J.C.
University of Chicago, Chicago, IL (United States)

Lill, J.V.
University of Chicago, Chicago, IL (United States)

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

COMPLETION DATE - 09/01/1981 **PUBLICATION DATE** - 03/02/1992

DESCRIPTION - VIVAS2 computes the scattering S-matrix and transition probabilities for the collision of an S-state atom, A, with a sigma-state diatomic molecule, BC.

PACKAGE CONTENTS - NESC Note; Software Abstract; Program Documentation for VIVAS version II; Media Includes Source, Sample Problems;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

METHOD OF SOLUTION - The scattering S-matrix and transition probabilities are obtained by using either the variable interval variable step method, the log derivative method, or preferably a combination of both.

COMPUTER - DEC VAX11/780

OPERATING SYSTEMS - VMS 2.4

PROGRAMMING LANGUAGES - FORTRAN 77

SOFTWARE LIMITATIONS - Maxima of 600 quantum states for the system, 300 rotational J values, 150 channels to be integrated, 50 oscillator basis functions, and 50 vibrational states. The S-matrix analysis assumes that there are no coulomb interactions.

SOURCE CODE AVAILABLE (Y/N) - Y

RELATED SOFTWARE - VIVAS2 incorporates the log derivative method of the LOGD program and supersedes the VIVAS program which was transferred in February 1981 from the National Resource for Computation in Chemistry's software library.

OTHER PROG/OPER SYS INFO - The values of the parameters, NCHAN and NCHRMT, in subroutine SCATTR can be changed from 150 to 50 to

PACKAGE ID - 000265D078000 VIVAS2

OTHER PROG/OPER SYS INFO - (CONT) reduce machine requirements for execution to 1.1 megabytes if size is a problem. Subroutine FMPTIM must be supplied by the user. This routine returns the current wall clock time in the form hh:mm:ss, where hh,mm, and ss are hours, minutes, and seconds, respectively.

HARDWARE REQS - 2.9 megabytes of memory are required to execute the sample problems.

TIME REQUIREMENTS - NESC executed each sample problem in less than 30 CPU seconds on a DEC VAX11/780.

REFERENCES - G.A. Parker, Program Documentation for VIVAS version II, August 10, 1981; VIVAS2, NESC No. 966.VX11, VIVAS2 Tape Description and Implementation Information, National Energy Software Center Note 82-38, January 22, 1982; Gregory A. Parker, Thomas G. Schmalz, and John C. Light, A variable interval variable step method for the solution of linear second order coupled differential equations, Journal of Chemical Physics, Vol. 73, No. 4, 1980; Gregory A. Parker and John C. Light, The Logarithmic Derivative-Variable Interval Variable Step Hybrid Method for the Solution of Coupled Linear Second-Order Differential Equations, Chemical Physics Letters, Vol. 73, No. 3, 1980; Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume I, Proceedings of the Workshop Held at Argonne National Laboratory, June 25-27, 1979, CONF-790696 (LBL-9501), Vol. I, NRCC Proceedings No. 5, July 1980; Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume II, Proceedings of the Workshop Reconvened at Lawrence Berkeley Laboratory, October 26-27, 1979, CONF-790696 (LBL-9501), Vol. II, NRCC Proceedings No. 5, July 1980; L.D. Thomas, M.H. Alexander, B.R. Johnson, W.A. Lester, Jr., J.C. Light, K.D. McLenithan, G.A. Parker, M.J. Redmon, T.G. Schmalz, D. Secrest, and R.B. Walker, Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory, Journal of Computational Physics, Vol. 41, No. 2, pp. 407-426, June 1981, also available as LBL-11233, July 1980.

ABSTRACT STATUS - Abstract first distributed April 1982. DEC VAX11/780 version submitted September 1981, sample problems executed by NESC January 1982 on a DEC VAX11/780.

SUBJECT CLASS CODE - W

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
V CODES
TRANSITION AMPLITUDES
ATOM-MOLECULE COLLISIONS
S MATRIX
SCATTERING

E S T S C
ENERGY SCIENCE & TECHNOLOGY SOFTWARE CENTER
SOFTWARE ABSTRACT

PAGE 3
DATE 03/13/2002

PACKAGE ID - 000265D078000 VIVAS2

SCHROEDINGER EQUATION

EDB SUBJECT CATEGORIES -
990200 664300

SPONSOR - DOE/ER

PACKAGE TYPE - TESTED