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Form Approved
OMB No. 0704-0188

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2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; Distribution is unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR- 89-0074
6a. NAME OF PERFORMING ORGANIZATION: Florida A&M University 6b. OFFICE SYMBOL (If applicable):	7a. NAME OF MONITORING ORGANIZATION: AFOSR/NC
6c. ADDRESS (City, State, and ZIP Code): Department of Physics, Tallahassee, FL 32307	7b. ADDRESS (City, State, and ZIP Code): Building 410, Bolling AFB, DC 20332-6448
8a. NAME OF FUNDING/SPONSORING ORGANIZATION: AFOSR 8b. OFFICE SYMBOL (If applicable): NC	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: AFOSR-86-0149
8c. ADDRESS (City, State, and ZIP Code): Building 410, Bolling AFB, DC 20332-6448	10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO.: 61102F PROJECT NO.: 2303 TASK NO.: B3 WORK UNIT ACCESSION NO.:

11. TITLE (Include Security Classification)
Analytic Methods Using Computer Algebra with Slater-Type Orbitals for Problems in AB Initio Quantum Chemistry and Molecular Physics

12. PERSONAL AUTHOR(S)
H. W. JOnes, and C. A. Weatherford

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
FINAL	FROM 5-1-86 TO 9-30-88		3

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

See Back

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☒ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS	UNCLASSIFIED

22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE (Include Area Code)	22c. OFFICE SYMBOL
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DD Form 1473, JUN 86 — Previous editions are obsolete. — SECURITY CLASSIFICATION OF THIS PAGE

19. **Our chief concern is the production of a STO (Slater-type orbital) integral package with application to diatomic and polyatomic molecules and ions by use of the "Columbus Codes". Comparisons are to be made with GTO (Gaussian-type orbital) codes. We feel confident that the superiority of STOs over GTOs will be most pronounced for excited states and multiple moments using inverse powers of the radial distance. Our judicious use of integer arithmetic and expansions in Taylor series should bring success to the elusive goal. The outline of this new strategy is presented in a recent paper: "Analytical Evaluation of Multicenter Molecular Integrals Over Slater-Type Orbitals Using Expanded Lowdin Alpha Functions". Work on electron scattering continues to move at a rapid pace. The finite difference method has gained international recognition with Dr. Weatherford's presentation of his results at a conference in Italy and the presentation at the ICPEAC meeting in London by his collaborator, Dr. Temkin. Naturally, we hope to combine this method with STOs.**

AFOSR-TR- 89-0074

Final Technical Report
Period: May 1, 1986 - September 30, 1989
Grant No. AFOSR - 86-0149

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PAPERS PUBLISHED AND WRITTEN

1. H.W. Jones, "Exact formulas and their evaluation for Slater-type orbital overlap integrals with large quantum numbers", Phys. Rev. A, 35, 1923 (1987).

2. H.W. Jones, B. Bussery, and C.A. Weatherford, "An E-Matrix for the Löwdin Alpha-function, Expanded in a Taylor Series: An Analytic Treatment of Molecular Charge Density Near the Origin", Int. Journal of Quantum Chem. 21, 693 (1987).

3. H.W. Jones, Progress Report. "The Exponential Integral Function Ei Computed to Specified Accuracy".

4. C.A. Weatherford, F.B. Brown, and A. Temkin, "Inclusion of Electron Correlation for the Target Wave Function in Low to Intermediate Energy e-N_2 Scattering", Phys. Rev. A, 35, 4561 (1987).

5. C.A. Weatherford, "An Analytic Method for the Three-center Nuclear Attraction Integral: A Generalization of the Gegerbauer Addition Theorem", Int. Journal of Quantum Chemistry 33, 19 (1988).

6. H.W. Jones, "Analytical evaluation of multicenter molecular integrals over Slater-type orbitals using expanded Löwdin alpha functions, Phys. Rev. A, 38, 1065 (1988).

7. H.W. Jones, B. Etemadi, C.A. Weatherford, "Analytical Evaluation of the Electrostatic Potential for Diatomic Molecules", Int. J. Quantum Chem. (To be published).