

ALGORITHM 104 REDUCTION TO JACOBI

H. RUTISHAUSER

Eidg. Technische Hochschule, Zurich, Switzerland

procedure *m21* (*n*, *a*, *b*, *c*, *inform*); **value** *n*;
integer *n*; **array** *a*, *b*, *c*; **procedure** *inform*;
comment: *m21* transforms symmetric bandmatrix

$$\begin{pmatrix} a[1] & b[1] & c[1] & & & \\ b[1] & a[2] & b[2] & c[2] & & \\ c[1] & b[2] & a[3] & b[3] & & \\ & c[2] & & & c[n-2] & \\ & & & & a[n-1] & b[n-1] \\ & & & & c[n-2] & b[n-1] & a[n] \end{pmatrix}$$

represented by the arrays *a*, *b*, *c* by orthogonal transformation to Jacobi form which is represented by the arrays *a*, *b*. The method is described in H. RUTISHAUSER, "On Jacobi rotation patterns," to appear in Proc. Symposium in Experimental Arithmetic, Chicago, Apr. 12-14, 1962, Sect. 5. Note that declarations must be given for the arrays *a*, *b*, *c* with subscripts ranging from 1 to *n*. Also procedure *inform* must be declared. It may serve to use the Jacobi rotations occurring inside *m21* also for other purposes;

```
begin
  real p, g, d, s;
  integer k, j;
  b[n] := c[n] := c[n-1] := 0;
  for k := 2 step 1 until n-1 do
    begin
      for j := k step 2 until n-1 do
        begin
          if k=j then
            begin
              p := sqrt(b[k-1]2 + c[k-1]2);
              if p=0 then go to ex;
              d := b[k-1]/p;
              s := -c[k-1]/p;
              b[k-1] := p;
              c[k-1] := 0;
            end k=j
          else
            begin
              p := sqrt(c[j-2]2 + g2);
              if p = 0 then go to ex;
              d := c[j-2]/p;
              s := -g/p;
              c[j-2] := p;
              p := d×b[j-1] - s×c[j-1];
              c[j-1] := s×b[j-1] + d×c[j-1];
              b[j-1] := p
            end j≠k;
          common: g := 2×b[j]×d×s;
              p := a[j]×d×d - g + a[j+1]×s×s;
              b[j] := (a[j] - a[j+1])×d×s + b[j]×(d×d - s×s);
              a[j+1] := a[j]×s×s + g + a[j+1]×d×d;
              a[j] := p;
              p := d×c[j] - s×b[j+1];
              b[j+1] := s×c[j] + d×b[j+1];
              c[j] := p;
              g := -s×c[j+1];
              c[j+1] := d×c[j+1];
            inform (n, j, d, s);
          comment: The Jacobi rotation which has been performed
```

Algorithms

J. H. WEGSTEIN, Editor

in this turn of the *j*-loop is $A := U^T A U$ with

$$U = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & d & s & \\ & & -s & d & \\ & 0 & & & 1 \end{pmatrix},$$

where the *d*'s and *s*'s are located at the crosspoints of rows and columns *j* and *j* + 1;

```
end j;
ex: end k
end m21
```

ALGORITHM 105

NEWTON MAEHLY

F. L. BAUER AND J. STOER

Johannes Gutenberg-Universität, Mainz, Germany

```
procedure Newton Maehly (a, n, z, eps);
  value n, eps;
  array a, z;
  integer n;
  real eps;
  comment The procedure determines all zeros z[1:n] of the
    polynomial  $p(x) := a[0] \times x^n + \dots + a[n]$  of order n, if p(x)
    has only real zeros which have to be all different. The zeros
    z[i] are ordered according to their magnitude: z[1] > z[2] >
    ... > z[n]. The approximations for each zero will be improved
    by iteration as long as  $\text{abs}(x_1 - x_0) > \text{eps} \times \text{abs}(x_1)$  holds
    for two successive approximations x0 and x1;
  begin real aa, pp, qq, x0, x1;
    integer i, m, s;
    array b, p, q[0:n-1];
    procedure Horner(p, q, n, x, pp, qq);
      value n, x;
      array p, q;
      real pp, x, qq;
      integer n;
      begin real s, s1;
        integer i;
        s := s1 := 0;
        for i := 0 step 1 until n-1 do
          begin s := s×x + p[i]; s1 := s1×x + q[i]; end;
          pp := s×x + p[n]; qq := s1;
        end;
        p[0] := aa := a[0]; x0 := pp := 0; s := sign(a[0]);
        for i := 1 step 1 until n do
          if s × a[i] < 0 then
            begin if pp=0 then pp := i;
              if x0 < abs(a[i]) then x0 := abs(a[i]);
            end;
            x0 := if pp=0 then 0 else 1 + exp(ln(abs(x0/aa))/pp);
          comment x0 is a first approximation for the largest zero which
            may be printed out at this point of the program;
          for i := 0 step 1 until n-1 do b[i] := (n-1)×a[i];
```

```

for m := 1 step 1 until n do
  begin
    iteration:
      Horner (a, b, n, x0, pp, qq); x1 := x0 - pp/qq;
      if abs(x1 - x0) > eps × abs(x1) then
        begin x0 := x1;
          comment x0 is the last approximation for the zero
            being improved, which may be printed out at this
            point;
          go to iteration;
        end;
      z[m] := x1;
      comment z[m] := x1 is the mth zero of the polynomial;
      pp := b[0] := b[0] - aa; q[0] := pp;
      if m < n then
        begin for i := 1 step 1 until n-1 do
          begin pp := p[i] := x1 × p[i-1] + a(i);
            pp := b[i] := b(i) - pp;
            q[i] := x1 × q[i-1] + pp;
          end;
          Horner (p, q, n-1, x1, pp, qq);
          x0 := x1 - pp/qq;
          comment x0 is a first approximation for the
            next zero;
        end
      end
    end Newton Maehly;
  end

```

ALGORITHM 106

COMPLEX NUMBER TO A REAL POWER

MARGARET L. JOHNSON AND WARD SANGREN

Computer Applications, Inc., San Diego, California

```

procedure POWC (x, y, w, A, B); value x, y, w;
  real x, y, w, A, B;
  comment This procedure takes a complex number  $(x+iy)$  to
    a real power  $w$ . The result is  $A+iB = (x+iy)^w$ . This procedure
    must be used with caution because although it is formally cor-
    rect, it may not give the desired results. For example, if  $w$  is a
    reciprocal integer it does not follow that the desired power
    (a root) will be calculated;
  begin real THETA, PHI, R;
    if x > 0 then begin THETA := 0.0; go to SOL 1 end;
    if x < 0 ∧ y ≥ 0 then begin THETA := 3.1415927;
      go to SOL 1 end;
    if x < 0 ∧ y < 0 then begin THETA := 3.1415927;
      go to SOL 1 end;
    if x = 0 ∧ y = 0 then begin A := B := 0.0; go to RETURN end;
    if x = 0 ∧ y < 0 then begin PHI := 1.5707963; go to SOL 2 end;
    if x = 0 ∧ y > 0 then begin PHI := -1.5707963;
      go to SOL 2 end;
    SOL 1: PHI := arctan (y/x) + THETA;
    SOL 2: R := sqrt (x×x+y×y);
      R := exp (w×ln(R));
      A := R×cos (w×PHI);
      B := R×sin (w×PHI);
    RETURN: end POWC

```

ALGORITHM 107

GAUSS'S METHOD

JAY W. COUNTS

University of Missouri, Columbia, Mo.

```

procedure gauss (u, a, y);
  real array a, y; real temp; integer u;

```

comment This **procedure** is for solving a system of linear equations by successive elimination of the unknowns. The augmented matrix is a and u the number of unknowns. The solution vector is y . If the system hasn't any solution or many solutions, this is indicated by **go to stop**;

```

  begin
    integer i, j, k, m, n;
    n := 0;
  ck0: n := n+1;
    for k := n step 1 until u do if a[k, n] ≠ 0 then go to ck1;
    go to stop;
  ck1: if k = n then go to ck2;
    for m := n step 1 until u+1 do
      begin
        temp := a[n, m]; a[n, m] := a[k, m]; a[k, m] := temp
      end;
  ck2: for j := u+1 step -1 until n do a[n, j] := a[n, j]/a[n, n];
    for i := k+1 step 1 until u do
      for j := n+1 step 1 until u+1 do
        a[i, j] := a[i, j] - a[i, n] × a[n, j];
      if n ≠ u then go to ck0;
      for i := u step -1 until 1 do
        begin
          y[i] := a[i, u+1]/a[i, i];
          for k := i-1 step -1 until 1 do
            a[k, u+1] := a[k, u+1] - a[k, i] × y[i]
          end end;

```

ALGORITHM 108

DEFINITE EXPONENTIAL INTEGRALS A

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

```

real procedure As (n, b); value n, b; integer n; real b;
  comment: This procedure computes a value of integral
     $A_{n-1}(1, b) = \int_1^{\infty} x^{n-1} \exp(-bx) dx$  for any given positive integer,  $n$ ,
    and any positive real parameter,  $b$ , by the recursion formula
     $A_n(1, b) = A_0(1, b) + (n/b)A_{n-1}(1, b)$  with  $A_0(1, b) = \exp(-b)/b$ ;
  begin integer m; real db; real array a[1:n];
    a[1] := exp (-b)/b;
    if n = 1 then go to exit;
  comment integral  $a[1] = A_0(1, b)$  was evaluated;
    db := 1/b; for m := 2 step 1 until n do a[m] :=
      a[1] + db × (m-1) × a[m-1];
  comment integral  $a[n] = A_{n-1}(1, b)$  was evaluated;
    As := a[n] end As;

```

ALGORITHM 109

DEFINITE EXPONENTIAL INTEGRALS B

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

```

real procedure Bs(n, a); value n, a; integer n; real a;
  comment This procedure computes a value of the integral
     $B_{n-1}(a) = \int_{-1}^1 x^{n-1} \exp(-ax) dx$  for any given positive integer,  $n$ ,
    and any real parameter,  $a$ . If  $|a| < \text{alim}$  an expansion of
     $\exp(-ax)$  is used, otherwise the recursion formula  $B_n(a) =$ 
     $[(-1)^n e^a - e^{-a} + nB_{n-1}(a)]/a$  with  $b_0(a) = 2 \sinh(a)/a$  is used. The
    value of alim depends upon the highest  $n$  appearing in the

```

calculations and upon the maximum errors in the last significant digits in the library procedures. For example, we have used $\text{alim}=8$ for $n_{\max}=16$ with $\text{gamma}=1 \times 10^{-8}$. The intrinsic function $\text{mod}(E_1, E_2)$ which requires two integer arguments, is the conventional modulus;

```

begin    integer m; real alim, delta, gamma, r, epsilon,
          s, k, a2, omega, da, jp, jm, q1, q2; real array
          b[1:n]; if a=0 then
L1:      begin if  $\text{mod}(n-1, 2)=0$  then
L2:      begin  $b[n] := 2/n$ ; go to exit end L2;
comment integral  $b[n] = B_{n-1}(0)$  for odd  $n$  was evaluated;
           $b[n] := 0$ ; go to exit end L1;
comment integral  $b[n] = B_{n-1}(0)$  for even  $n$  was evaluated;
          if  $\text{abs}(a) \text{ alim}$  then
L3:      begin  $\text{delta} := \text{gamma}$ ; if  $\text{mod}(n-1, 2)=0$  then
L4:      begin  $r := 2/n$ ;  $\text{epsilon} := r \times \text{delta}$ ;  $s := r$ ;
           $k := 0$ ;  $a2 := a^2$ ;
Even:     $k := k+2$ ;
           $r := r \times a2 \times (n+k-2)/(k \times (k-1) \times (n+k))$ ;
           $s := s+r$ ; if  $r > \text{epsilon}$  then go to Even;
           $b[n] := s+r$ ;
          go to exit end L4;
comment integral  $b[n] = B_{n-1}(a)$  for odd  $n$  and  $|a| < \text{alim}$  was
          evaluated;
           $r := 2 \times a/(n+1)$ ;  $\text{omega} := \text{abs}(r \times \text{delta})$ ;
           $s := r$ ;  $k := 1$ ;
           $a2 := a^2$ ;
Odd:      $k := k+2$ ;
           $r := r \times a2 \times (n+k-2)/(k \times (k-1) \times (n+k))$ ;
           $s := s+r$ ; if  $\text{abs}(r) > \text{omega}$  then go to Odd;
           $b[n] := -(s+r)$ ; go to exit end L3;
comment integral  $b[n] = B_{n-1}(a)$  for even  $n$  and  $|a| < \text{alim}$  was
          evaluated;
           $da := 1/a$ ;  $jp := da \times \exp(a)$ ;  $jm := (da^2)/jp$ ;
           $b[1] := jp - jm$ ;
          if  $n=1$  then go to exit;
comment integral  $b[1] = B_0(a)$  for  $|a| \geq \text{alim}$  was evaluated;
           $q1 := -1$ ;  $q2 := 1$ ; for  $m := 2$  step 1 until  $n$  do
L5:      begin  $b[m] := q1 \times jp - jm + q2 \times da \times b[m-1]$ ;
           $q1 := -q1$ ;  $q2 := q2+1$  end L5;
comment integral  $b[n] = B_{n-1}(a)$  for integer  $n \geq 2$  and  $|a| \geq \text{alim}$ 
          was evaluated;
exit:     $Bs := b[n]$  end Bs;

```

ALGORITHM 110

QUANTUM MECHANICAL INTEGRALS OF SLATER-TYPE ORBITALS

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

real procedure INTSOLI (n, r, za, ab, As, Bs) **Result:**
 $(s, i1, i2, i3)$; **value** n, r, za, zb ; **integer** n ; **real** r, za, zb ;
real array $a[1:8], b[1:8], G[1:2 \times n]$; **integer array** $bc[1:2 \times n,$
 $1:2 \times n]$; **real procedure** As, Bs ;

comment Procedure INTSOLI computes the quantum mechanical integrals $s = \langle \psi_{n00}^{ai} | \psi_{210}^{bi} \rangle$ (overlap integral),
 $i1 = \langle \psi_{n00}^{ai} | Z_a^*/r_{ai} | \psi_{210}^{bi} \rangle$ (exchange integral),
 $i2 = \langle \psi_{n00}^{ai} | Z_b^*/r_{bi} | \psi_{n00}^{ai} \rangle$ (coulomb integral),
and $i3 = \langle \psi_{210}^{bi} | Z_a^*/r_{ai} | \psi_{210}^{bi} \rangle$ (coulomb integral).

Here $|\psi_{nlm}^{ai}\rangle$ is a Slater-type orbital of electron i centered on atomic nucleus a . The integer n is the effective principal quantum number with values 1, 2, 3 and 4. $Z_a^* = za$ and $Z_b^* = zb$ are effective nuclear charges. r_{bi} is the distance of electron

i from nucleus b . The input parameter r is the distance between the two centers a and b . All physical quantities are given in atomic units;

```

begin    integer q, t, c, m;
          real g, zsa, zsb, ks, p, pt, lilya, s, k1, exc, i1, pppt,
          k2, sue, i2, pmpt, ptmp, k3, i3;
           $bc[1, 1] := bc[2, 1] := bc[2, 2] := 1$ ;
          for  $q := 3$  step 1 until  $2 \times n$  do
L6:      begin  $bc[g, 1] := 1$ ; for  $t := 2$  step 1 until  $g-1$  do
           $bc[q, t] := bc[q-1, t-1] + bc[q-1, t]$ ;
           $bc[q, q] := 1$  end L6;
comment binomial coefficients  $bc[q, t] = \binom{q-1}{t-1}$  were computed
          using the recursion formula  $\binom{q}{t} = \binom{q-1}{t-1} + \binom{q-1}{t}$ ;
procedure  $As(n, b)$  Result:  $(a[n])$ ; value  $n, b$ ; integer  $n$ ;
          real  $b$ ;
comment procedure  $As$  computes a value of integral  $A_{n-1}(1, b)$ 
          [see Algorithm 108, "Definite Exponential Integrals  $A$ ," by Yuri A. Kruglyak and D. R. Whitman, Comm. ACM (July 1962)]. Any identifier occurring
          within the  $As$  is specified to be local to the  $As$ ;
begin    integer  $m$ ; real  $db$ ;  $a[1] := \exp(-b)/b$ ;
          if  $n=1$  then go to exitAs;  $db := 1/b$ ;
          for  $m := 2$  step 1 until  $n$  do  $a[m] := a[1] +$ 
           $db \times (m-1) \times a[m-1]$ 
exitAs: end  $As$ ;
procedure  $Bs(n, a)$  Result:  $(b[n])$ ; value  $n, a$ ; integer  $n$ ;
          real  $a$ ;
comment procedure  $Bs$  computes a value of integral  $B_{n-1}(a)$ 
          [see Algorithm 109, "Definite Exponential Integrals  $B$ ," by Yuri A. Kruglyak and D. R. Whitman, Comm. ACM (July 1962)]. Any identifier occurring
          within the  $Bs$  is specified to be local to the  $Bs$ ;
begin    integer  $m$ ; real  $\text{alim}, \text{delta}, \text{gamma}, r, \text{epsilon},$ 
           $s, k, a2, \text{omega}, da, up, jm, q1, q2$ ;
          if  $a=0$  then begin if  $\text{mod}(n-1, 2)=0$ 
          then begin  $b[n] := 2/n$ ; go to exitBs end;
           $b[n] := 0$ ; go to exitBs end;
          if  $\text{abs}(a) < \text{alim}$  then begin  $\text{delta} := \text{gamma}$ ;
comment we have used  $\text{alim}=8$  and  $\text{gamma}=1 \times 10^{-8}$ ;
          if  $\text{mod}(n-1, 2)=0$  then begin  $r := 2/n$ ;
           $\text{epsilon} := r \times \text{delta}$ ;
           $s := r$ ;  $k := 0$ ;  $a2 := a^2$ ;
Even:     $k := k+2$ ;
           $r := r \times a2 \times (n+k-2)/((k \times (k-1) \times (n+k)))$ ;
           $s := s+r$ ; if  $r > \text{epsilon}$  then go to Even;
           $b[n] := s+r$ ;
          go to exitBs end;  $r := 2 \times a/(n+1)$ ;
           $\text{omega} := \text{abs}(r \times \text{delta})$ ;
           $s := r$ ;  $k := 1$ ;  $a2 := a^2$ ;
Odd:      $k := k+2$ ;
           $r := r \times a2 \times (n+k-2)/(k \times (k-1) \times (n+k))$ ;
           $s := s+r$ ; if  $\text{abs}(r) > \text{omega}$  then go to Odd;
           $b[n] := -(s+r)$ ; go to exitBs end;  $da := 1/a$ ;
           $jp := da \times \exp(a)$ ;
           $jm := (da^2)/jp$ ;  $b[1] := jp - jm$ ;
          if  $n=1$  then go to exitBs;
           $q1 := -1$ ;  $q2 := 1$ ; for  $m := 2$  step 1 until  $n$ 
          do begin  $b[m] := q1 \times jp - jm + q2 \times da \times b[m-1]$ ;
           $q1 := -q1$ ;  $q2 := q2+1$  end
exitBs: end  $Bs$ ;
           $g := 1$ ; for  $m := 1$  step 1 until  $2 \times n$  do  $g := g/m$ ;
           $G[2 \times n] := g$ ;
comment  $1/(2n)! = G[2 \times n]$  was evaluated;
           $zsa := za/n$ ;  $zsb := zb/2$ ;  $ks := (r/2)^{\uparrow(n+3)} \times$ 
           $(2 \times zsa)^{\uparrow(n+1/2)} \times zsb^{\uparrow(5/2)} \times G[2 \times n]^{\uparrow(1/2)}$ ;
           $p := r \times (zsa + zsb)/2$ ;

```

```

pt := r×(zsa-zsb)/2;
  for c := 1 step 1 until n+3 do
ABSI:   begin As(c, p) Result: (a[c]);
        Bs(c, pt) Result: (b[c])
  end ABSI;
S:      lilya := 0; for m := 0 step 1 until n do lilya :=
        lilya+bc[n+1, m+1]×(a[n-m+2]×(b[m+1]+
        b[m+3])−b[m+2]×(a[n-m+1]+a[n-m+3]));
        s := ks×lilya;
I1:     k1 := ks×2×za/r; exc := 0;
        for m := 0 step 1 until n-1 do
exc := exc+bc[n, m+1]×(a[n-m+1]×(b[m+1]+
        b[m+3])−b[m+2]×(a[n-m]+a[n-m+2]));
        il := k1×exc;
I2:     pppt := p+pt; k2 := (r/2)↑(2×n)×(2×zsa)↑
        (2×n+1)×zsb×G[2×n];
        for c := 1 step 1 until 2×n do
BA2:   begin As(c, pppt) Result: (a[c]);
        Bs(c, pppt) Result: (b[c])
  end BA2; sue := 0;
        for m := 0 step 1 until 2×n-1 do
sue := sue+bc[2×n, m+1]×a[2×n-m]×b[m+1];
        i2 := k2×sue;
I3:     pmpt := p-pt; ptmp := -pmpt;
        k3 := (r/2)↑4×2×za×zsb↑5;
        for c := 1 step 1 until 4 do
AB3:   begin As(c, pmpt) Result: (a[c]);
        Bs(c, ptmp) Result: (b[c])
  end AB3; i3 := k3×(a[2]×(b[1]+2×b[3])−b[2]×
        (a[1]+2×a[3])+a[4]×b[3]−a[3]×b[4]) end
INTSOLI;

```

ALGORITHM 111 MOLECULAR-ORBITAL CALCULATION OF MOLECULAR INTERACTIONS

YURI A. KRUGLYAK
Kharkov State University, Kharkov, U.S.S.R., AND
DONALD R. WHITMAN
Case Institute of Technology, Cleveland, Ohio

real procedure SOLI(n, za, zb, rem, coef2, r1, E1, dr1, drk1, acc, acc1, rk2, rk1, dr2, asy, rk3, dr3, As, Bs, RESULT) Result: (ra, Ep, Em, ca, ca2, cb, cb2, DEa, DEb, s, i1, i2, i3, haa, hab, hbb); **value** n, za, zb, rem, coef2, r1, E1, dr1, rk1, drk1, acc, acc1, rk2, dr2, asy, rk3, dr3; **integer** n, rem; **real** otherwise; **real array** a[1:8], b[1:8], G[1:8], zsa [1:9], rp[1:8], ans[1:rem]; **real procedure** As, Bs, RESULT;

comment This procedure calculates a one-electron approximation to the energy of interaction of molecular species by the use of the molecular-orbital (MO) method with a linear combination of Slater-type orbitals (LCSTO). The wave function used is $|\phi\rangle = c_a |\psi_{n00}^a\rangle + c_b |\psi_{210}^b\rangle$, where $|\psi_{nlm}^a\rangle$ is a STO centered on nucleus a . The effective principal quantum number n takes the integral value 1, 2, 3 or 4. The Hamiltonian used is: $\mathcal{H}_{ab} = -\Delta/2 - Z_a^*/r_a - Z_b^*/r_b + Z_a^*Z_b^*/R_{ab}$. Here Z_a^* and Z_b^* are effective nuclear charges, r_a and r_b the distances of the electron from nucleus a and b , and R_{ab} is the distance between nuclei a and b . The calculations are in atomic units, while the output ra is in Angstroms and DEa and DEb are in kcal/gm-ion. Abbreviations of the following type are used: $Za = Z_a^*$, $ra = R_{ab}(\text{\AA})$, $haa = \langle \psi_{n00}^a | \mathcal{H}_{ab} | \psi_{n00}^a \rangle$, $DEa = D(a, b + \text{electron})$, $e1 = \langle \psi_{n00}^a | -\Delta/2 - Z_a^*/r_a | \psi_{n00}^a \rangle$. The values of coef1 and coef2 are 627.71 (kcal/gm-ion) and 0.5291 $\text{\AA}$, respectively. $r1$, $E1$, $dr1$, $dr2$, $dr3$, acc , $acc1$, and asy are control parameters. The accuracy of the calculations (acc , $acc1$) is 1×10^{-5} . The

initial values of R_{ab} and E_1 are conveniently: $r1 = 0.4(\text{\AA})$, and $E1 = 100(\text{a.u.})$. The steps are: $dr1 = 0.1$, $dr2 = 0.4$, and $dr3 = 0.01$, all in Angstroms. asy is $-1 \times 10^{-3}(\text{a.u.})$;

```

begin   integer q, t, c, m, f; real otherwise;
procedure As(n, b) Result: (a[n]); value n, b; integer n;
        real b;
comment any identifier occurring within the As is specified
        to be local to the As;
begin   integer m; real db; a[1] := exp(-b)/b;
        if n=1 then go to exitAs; db := 1/b;
        for m := 2 step 1 until n do a[m] := a[1]+db×
        (m-1)×a[m-1]
exitAs: end As;
procedure Bs(n, a) Result: (b[n]); value n, a; integer n;
        real a;
comment any identifier occurring within the Bs is specified
        to be local to the Bs;
begin   integer m; real otherwise; if a=0 then begin if
        mod(n-1, 2)=0 then begin b[n] := 2/n;
        go to exitBs end; b[n] := 0; go to exitBs end;
        if abs(a)<alim then begin delta := gamma;
        if mod(n-1, 2)=0 then begin r := 2/n;
        epsilon := r×delta; s := r; k := 0; a2 := a↑2;
Even:   k := k+2; r := r×a2×(n+k-2)/(k(k-1)(n+k));
        s := s+r; if r>epsilon then go to Even;
        b[n] := s+r; go to exitBs end;
        r := 2×a/(n+1); omega := abs(r×delta);
        s := r; k:=1; a2 := a↑2;
Odd:   k := k+2; r := r×a2×(n+k-2)/(k(k-1)(n+k));
        s := s+r; if abs(r)>omega then go to Odd;
        b[n] := -(s+r); go to exitBs
end; da := 1/a; jp := da×exp(a);
        jm := (da↑2)/jp; b[1] := jp-jm;
        if n=1 then go to exitBs; q1 := -1; q2 := 1;
        for m := 2 step 1
        until n do begin b[m] := q1×jp-jm+
        q2×da×b[m-1];
        q1 := -q1; q2 := q2+1 end
exitBs: end Bs;
procedure Result(coef1); real coef1;
comment RESULT computes Ep, Em, ca, ca2, cb, cb2, DEa,
        DEb, s, i1, i2, i3, nn, haa, hab, hbb. Important:
        RESULT and any identifier occurring within the
        RESULT enter SOLI as nonlocal entities;
begin   r := ra×br; rp[1] := r; for c := 2 step 1 until
        n+4 do rp[c] := rp[c-1]×rp[1]; p := r×sum;
        pt := r×dif; ks := rp[n+3]×zss;
        for c:= 1 step 1 until n+3 do begin As(c, p)
        Result: (a[c]); Bs(c, pt) Result: (b[c]) end;
        lilya := 0; for m := 0 step 1 until n do lilya :=
        lilya+bc[n+1, m+1]×(a[n-m+2]×
        (b[m+1]+b[m+3])−b[m+2]×(a[n-m+1]
        +a[n-m+3])); s := ks×lilya; li12 := 2×s;
        k1 := ks×za/r; exc := 0; for m := 0 step 1
        until n-1 do exc := exc+bc[n, m+1]×(a[n-m
        +1]×(b[m+1]+b[m+3])−b[m+2]×(a[n-m]
        +a[n-m+2])); il := k1×exc; pppt := p+pt;
        k2 := rp[2×n]×zsb; for c := 1 step 1 until
        2×n do begin As(c, pppt) Result: (a[c]);
        Bs(c, pppt) Result: (b[c]) end; sue := 0;
        for m := 0 step 1 until 2×n-1 do sue :=
        sue+bc[2×n, m+1]×a[2×n-m]×b[m+1];
        i2 := k2×sue; pmpt := p-pt;
        ptmp := -pmpt; k3 := rp[4]×z5;
        for c := 1 step 1 until 4 do begin As(c, pmpt)
        Result: (a[c]); Bs(c, ptmp) Result: (b[c]) end;
        i3 := k3×(a[2]×(b[1]+2×b[3])−b[2]×(a[1]+2×
        a[3])+a[4]×b[3]−a[3]×b[4]);

```

comment Two-center integrals s , $i1$, $i2$, and $i3$ were computed [see Algorithm 110, "Quantum Mechanical Integrals of Slater-Type Orbitals," by Yuri A. Kruglyak and D. R. Whitman, *Comm. ACM* (July 1962)]; $nn := zz/(2 \times r)$; $e2pnn := e2 + nn$; $haa := e1 - e2 + nn$; $hbb := e2pnn - i3$; $hab := e2pnn \times s - i1$; $den := 2 - s \times li12$; $bsr := haa + hbb - hab \times li12$; $root := \sqrt{bsr^2 - 2 \times den \times (haa \times hbb - hab^2)}$; $Ep := (bsr + root)/den$; $Em := (bsr - root)/den$; $ans[f] := Em$; $DEa := coef1 \times (e2 - Em)$; $DEb := coef1 \times (e1 - Em)$; $Emhaa := Em - haa$; $Emhbb := Em - hbb$; $ES := Em \times s$; $habmES := hab - ES$; $caDecb1 := habmES/Emhaa$; $cbDca2 := habmES/Emhbb$; **if** $abs(Emhaa) > abs(Emhbb)$ **then begin** $col := caDecb1^2$; $cb2 := 1/(1 + li12 \times caDecb1 + col)$; $ca2 := cb2 \times col$; $ca := \sqrt{ca2}$; $cb := ca/caDecb1$ **go to NATA end**; $co2 := cbDca2^2$; $ca2 := 1/(1 + li12 \times cbDca2 + co2)$; $cb2 := ca2 \times co2$; $ca := \sqrt{ca2}$; $cb := ca \times cbDca2$
NATA: end RESULT;
 Begin of program: $bc[1, 1] := bc[2, 1] := bc[2, 2] := 1$;
for $q := 3$ **step 1 until 8 do begin** $bc[q, 1] := 1$; **for** $t := 2$ **step 1 until** $q-1$ **do** $bc[q, t] := bc[q-1, t-1] + bc[q-1, t]$; $bc[q, q] := 1$ **end**;
IZM: $g := 1$; **for** $m := 1$ **step 1 until** $2 \times n$ **do** $g := g/m$; $G[2 \times n] := g$; $zsa := za/n$; $zsap[1] := zsa \times 2$; **for** $c := 2$ **step 1 until** $2 \times n + 1$ **do** $xsap[c] := zsap[c-1] \times zsap[1]$; $D := zsap[2 \times n + 1] \times G[2 \times n]$; $DS := \sqrt{D}$; $e1 := -zsap[2] \times 0.125 \times (4 \times n - 3)/(2 \times n - 1)$; $zsb := zb \times 0.5$; $sum := zsa + zsb$; $dif := zsa - zsb$; $zsb5 := zsb^5$; $zss := DS \times \sqrt{zsb5}$; $zsbD := zsb \times D$; $z5 := 2 \times za \times zsb5$; $zz := za \times zb$; $e2 := -(zsb^2)/2$; $br := 0.5/coef2$; $f := 1$; $ans[1] := E1$; $ra := r1$;
KOM: $ra := ra + dr1$; **if** $ra > rk1$ **then** $ra := ra + drk1$; $f := f + 1$; **RESULT** ($coef1$); **if** $ans[f] - ans[f-1] \leq acc$ **then begin** **if** $ra > rk2$ **then go to IZM**; **go to KOM end**; $ansf := ans[f]$; $d1 := ra$;
CLEV: $ra := ra + dr2$; **RESULT** ($coef1$); **if** $e1 < e2$ **then begin** **if** $Em - e1 \leq asy \wedge ra < rk3$ **then go to CLEV**; **go to KHAR end**; **if** $e1 \geq e2$ **then begin** **if** $Em - e2 \leq asy \wedge ra < rk3$ **then go to CLEV**; **go to KHAR end**;
KHAR: $ra := d1$; $ansf[f-1] := ansf$;
CASE: $ra := ra - dr3$; $f := f + 1$; **RESULT** ($coef1$); **if** $ans[f] - ans[f-1] \leq acc1$ **then go to CASE**; **go to IZM end SOLI**;

REMARK ON ALGORITHM 34

GAMMA FUNCTION [M. F. Lipp, *Comm. ACM* 4 (Feb. 1961)]

MARGARET L. JOHNSON AND WARD SANGREN
 Computer Applications, Inc., San Diego, Calif.

The coefficients used in the calculation of the Hasting's polynomial are used in reverse order. The algorithm should have
 $a[1] = -.19352782$; $a[2] = .48219939$; $a[3] = -.75670408$;
 $a[4] = .91820686$; $a[5] = -.89705694$; $a[6] = .98820589$;
 $a[7] = -.57719165$; $a[8] = 1.0$;
 $y = .03586834$;

for $i := 1$ **step 1 until 8 do** $y := y \times x + a[i]$;

Further, since $\Gamma(x) = \Gamma(1+x)$, the divisor x in the statement labeled minus should be $x+1$.

REMARK ON ALGORITHM 48

LOGARITHM OF A COMPLEX NUMBER [John R. Herndon, *Comm. ACM* 4 (Apr. 1961)]

MARGARET L. JOHNSON AND WARD SANGREN
 Computer Applications, Inc., San Diego, Calif.

Considerable care must be taken in using the arctan function. In Algorithm 48 two such difficulties are ignored. First, it is necessary, because of a resulting division by zero, to deal separately with the case where the real part of the complex number is zero. Second, if the real part of the complex number is negative and the argument of the logarithm is to have a value between $-\pi$ and π then the action depends upon the sign of the imaginary part of the complex number. For clarity the following procedure exhibits in sequence the alternatives:

procedure LOGC (a, b, c, d); **value** a, b ; **real** a, b, c, d ;
comment This procedure computes the number $c+di$ which is equal to $\log_e(a+bi)$. It is assumed that the arctan has a value between $-\pi/2$ and $\pi/2$.
begin **if** $a > 0$ **then begin** $\theta := 0$; **go to SOL end**;
if $a < 0 \wedge b \geq 0$ **then begin** $\theta := 3.1415927$;
go to SOL end;
if $a < 0 \wedge b < 0$ **then begin** $\theta := -3.1415927$;
go to SOL end;
if $a = 0 \wedge b = 0$ **then begin** $c := d := 0$;
go to RETURN end;
if $a = 0 \wedge b > 0$ **then begin** $c := \ln(b)$; $d := 1.570963$;
go to RETURN end;
if $a = 0 \wedge b < 0$ **then begin** $c := \ln(abs(b))$;
 $d := 1.570963$; **go to RETURN end**;
SOL: $d := \arctan(b/a) + \theta$;
 $c := \sqrt{a^2 + b^2}$;
 $c := \ln(c)$;
RETURN: end LOGC

CERTIFICATION OF ALGORITHM 51

ADJUST INVERSE OF A MATRIX WHEN AN ELEMENT IS PERTURBED [John R. Herndon, *Comm. ACM* 4 (Apr. 1961)]

RICHARD GEORGE*

Argonne National Laboratory, Argonne, Ill.

This procedure was programmed in FORTRAN and reduced to machine code mechanically. It was run on the Argonne-built computing machine, GEORGE. A floating-point routine was used which allows maximum accuracy to 31 bits.

The procedure was tested for matrices with n ranging from 2 to 10. For each value of n , there were 20 successive trials; each trial consisted of a random perturbation of a randomly selected element of the matrix M , followed by a use of ADJUST, followed by the matrix multiplication $N := B \cdot M$. For each trial, the adjustment was evaluated by computing

$$\text{sum} := \left\{ \sum_{i=1}^n \sum_{j=1}^n N[i, j] \right\} - n.$$

For random perturbations between -1.0 and $+1.0$, the value of sum never exceeded $2.0_{10} - 8$.

There are two typographical errors present:

$B[r, s] = A[r, s] - t \times A[r, i] \times A[j, s]$ **end**

should be

$B[r, s] := A[r, s] - t \times A[r, i] \times A[j, s]$ **end**

* Work supported by the U. S. Atomic Energy Commission.

CERTIFICATION OF ALGORITHM 57
BER OR BEI FUNCTION [J. R. Herndon, *Comm. ACM*
4 (Apr. 1961)]

A. P. RELPH

The English Electric Co. Whetstone, England

Algorithm 57 was translated using the DEUCE ALGOL compiler.
No corrections were required, and the results were satisfactory.

CERTIFICATION OF ALGORITHM 70
INTERPOLATION BY AITKEN [C. J. Mifsud, *Comm.*
ACM 4 (Nov. 1961)]

A. P. RELPH

The English Electric Co., Whetstone, England

Algorithm 70 was translated using the DEUCE ALGOL compiler
and gave satisfactory results after semicolons had been added to

$t := j+1$ to make it $t := j+1$;

and $(x[i]-x[j])$ end to make it $(x[i]-x[j])$ end;

The identifier t can be eliminated and the algorithm shortened
by the following changes:

Replace **begin integer i, j, t;** by **begin integer i, j;**
Replace $t := j+1$; by **for i := j+1 step 1 until**
for i := t step 1 until n do
n do

CERTIFICATION OF ALGORITHM 75
FACTORS [J. E. L. Peck, *Comm. ACM* 5 (Jan. 1962)]

A. P. RELPH

The English Electric Co., Whetstone, England

Algorithm 75 was translated using the DEUCE ALGOL compiler
and gave satisfactory results after the following corrections had
been made:

begin if $q=0 \vee (an \div q) \times q = an$ **then**
begin if $q > 1 \wedge p=1$ **then**
was changed to
begin if $q \leq 1$ **then go to** NO CONSTANT;
if $(an \div q) \times q = an$ **then**
begin if $p=q$ **then**

begin $c := c \times a_0$; $a_0 := 1$
end

was changed to

begin $c := c \times a[0]$; $a[0] := 1$;
end

There are now r ($r > 0$) rational linear factors $(u_i x - v_i)$,
 $1 \leq i < r$,

was changed to

If $r > 0$ there are now r rational linear factors $(u_i x - v_i)$, $1 \leq i \leq r$,

To return to the state ($p=1, q=0$) after every factor or constant
is found is inefficient. This can be avoided by substituting $a[0]$
and $a[n]$ for the identifiers a_0 and a_n respectively. The procedure
then becomes:

```

procedure factors (n, a, u, v, r, c); value n, a;
integer array a, u, v;
integer r, n, c;
begin integer p, q;
  r := 0; c := 1;
ZERO: if  $a[n]=0$  then
  begin r := r+1; u[r] := 1; v[r] := 0; n := n-1;
  go to ZERO
  end;
for p := 1 step 1 until abs (a[0]) do
begin if  $(a[0] \div p) \times p = a[0]$  then
  begin for q := 1 step 1 until abs (a[n]) do
    begin if  $q=1$  then go to NO CONSTANT;
    TRY AGAIN: if  $(a[n] \div q) \times q = a[n]$  then
      begin integer j;
      for j := 0 step 1 until n-1 do
        if  $(a[j] \div q) \times q \neq a[j]$  then go to
        NO CONSTANT;
      for j := 0 step 1 until n do
         $a[j] := a[j]/q$ ;
      c := c×q; go to TRY AGAIN
    end;
    NO CONSTANT: begin integer f, g, i; f := a[0];
      g := 1;
      for i := 1 step 1 until n do
        begin g := g×p;
          f := f×q+a[i]×g
        end;
        if f=0 then
          begin r := r+1; u[r] := p;
            v[r] := q;
            begin integer i, t; t := 0;
            for i := 0 step 1 until n do
              begin  $a[i] := t := (a[i]+t)/p$ ;
                t := t×q
              end;
              n := n-1
            end
            go to if n=0 then REDUCED
              else NO CONSTANT
          end;
          q := -q; if  $q < 0$  then go to NO
            CONSTANT
        end
      end
    end
  end
  REDUCED: if n=0 then
    begin c := c×a[0]; a[0] := 1
    end
end

```

CERTIFICATION OF ALGORITHM 84
SIMPSON'S INTEGRATION [P. E. Hennion, *Comm.*
ACM 5 (Apr. 1962)]

A. P. RELPH

The English Electric Co., Whetstone, England

Simpson's Integration was translated using the DEUCE ALGOL
compiler and, with no corrections, gave satisfactory results.

It is not stated in the comment that integer n needs to be even.

CERTIFICATION OF ALGORITHM 108

DEFINITE EXPONENTIAL INTEGRALS A [Yuri A. Kruglyak and Donald R. Whitman, *Comm. ACM* 5 (July 1962)]

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R. and

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

Integrals $A_n(1, b) = \int_1^\infty x^n \exp(-bx) dx$ occur in physical problems involving spheroidal coordinates, particularly in quantum chemistry calculations. This algorithm was programmed for the Burrough's 220 computer using Burrough's Algebraic Compiler. The program was used to compute tables of $A_n(1, b)$ in the ranges $n=0(1)15$, and $b=0.01(0.01)30.14$. For example, for $n=0(1)15$, and $b=0.25$ and $b=24.0$, the results below were obtained. These are compared with the results (columns 3 and 5) obtained by James Miller, John M. Gerhauser, and F. A. Matsen [*Quantum Chemistry Integrals and Tables*, University of Texas Press, 1959].

n	$b=0.25$	$b=0.25$ (Miller et al.)	$b=24.0$	$b=24.0$ (Miller et al.)
0	.31152031, 01	.31152031322856, 01	.15729727, -11	.15729727267830, -11
1	.15576015, 02	.15576015661428, 02	.16385132, -11	.16385132570656, -11
2	.12772332, 03	.12772332842371, 03	.17095154, -11	.17095154982051, -11
3	.15357950, 04	.15357951442168, 04	.17866621, -11	.17866621640586, -11
4	.24575835, 05	.24575837510601, 05	.18707497, -11	.18707497541261, -11
5	.49151976, 06	.49151986541516, 06	.19627122, -11	.19627122588926, -11
6	.11796476, 08	.11796479885167, 08	.20636507, -11	.20636507915061, -11
7	.33030132, 09	.33030143989988, 09	.21748707, -11	.21748708743056, -11
8	.10569642, 11	.10569646079911, 11	.22979295, -11	.22979296848848, -11
9	.38050711, 12	.38050725887992, 12	.24346962, -11	.24346963586148, -11
10	.15220284, 14	.15220290355200, 14	.25874294, -11	.25874295428724, -11
11	.66969248, 15	.66969277562880, 15	.27588778, -11	.27588779339328, -11
12	.32145238, 17	.3214523320182, 17	.29524115, -11	.29524116937404, -11
13	.16715523, 19	.16715531679695, 19	.31721955, -11	.31721957275639, -11
14	.93606928, 20	.93606977406291, 20	.34234200, -11	.34234202345285, -11
15	.56164156, 22	.56164186443775, 22	.37126102, -11	.37126103733633, -11

The accuracy is at least six significant figures over the entire range. This accuracy is completely satisfactory for all quantum chemical calculations.

CERTIFICATION OF ALGORITHM 110

QUANTUM MECHANICAL INTEGRALS OF SLATER-TYPE ORBITALS [Yuri A. Kruglyak and Donald R. Whitman, *Comm. ACM* 5 (July 1962)]

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R. and

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

This procedure was written and tested in the Burroughs 220 version of the ALGOL language in the spring of 1961 at Case Institute of Technology. The program was used to compute tables of quantum mechanical integrals s , $i1$, $i2$, and $i3$ in the ranges: $r(\text{\AA})=0.64(0.02)1.40(0.10)3.10$; $Z_b^*=0.25(0.50)3.75$, 3.90 , 4.25 , 4.55 , 4.75 , 5.20 , 5.25 ; $Z_a^*=0.7$, 1.0 for $n=1$; $1.3(1.0)3.3$ for $n=2$; 0.2 , $2.2(1.0)4.2$ for $n=3$; and 0.2 , 2.2 , 3.2 for $n=4$. The table at the right shows typical results compared with values from *Integraltafeln zur Quantenchemie* by H. Preuss (Springer-Verlag, 1957), Zweiter Band. Accuracy is at least six significant figures in the ranges mentioned above. This is ample for the overwhelming majority of quantum chemistry calculations.

CERTIFICATION OF ALGORITHM 109

DEFINITE EXPONENTIAL INTEGRALS B [Yuri A. Kruglyak, D. R. Whitman, *Comm. ACM* 5 (July 1962)]

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., and

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

Integrals $B_n(a) = \int_{-1}^{+1} x^n \exp(-ax) dx$ occur in physical problems involving spheroidal coordinates, particularly in quantum chemistry calculations. This algorithm was programmed for the Burroughs-220 computer using a Burroughs Algebraic Compiler. The program was used to compute tables of $B_n(a)$ in the ranges $n=0(1)15$, and $a=0.00(0.01)32.54$. For example, for $n=0(1)15$ and $a=0.25$, and $a=24.0$ the results below were obtained. These are compared with the results (columns 3 and 5) obtained by James Miller, John M. Gerhauser, and F. A. Matsen [*Quantum Chemistry Integrals and Tables*, University of Texas Press, Austin, 1959].

n	$a=0.25$	$a=0.25$ (Miller et al.)	$a=24.0$	$a=24.0$ (Miller et al.)
0	.20208984, 01	.20208985344653, 01	.11037134, 10	.110371342208, 10
1	-.16771064, 00	-.16771066117520, 00	-.10577253, 10	-.105772536282, 10
2	.67921322, 00	.67921324506375, 00	.10155696, 10	.101556964184, 10
3	-.10074584, 00	-.10074585827159, 00	-.97676725, 09	-.976767216847, 09
4	.40896479, 00	.40896480211998, 00	.94091887, 09	.940918885936, 09
5	-.72008754, -01	-.72008756636929, -01	-.90768866, 09	-.907688654174, 09
6	.29268836, 00	.29268837517905, 00	.87679129, 09	.876791258533, 09
7	-.56030292, -01	-.56030294023170, -01	-.84798262, 09	-.847982638338, 09
8	.22792911, 00	.22792912573392, 00	.82105258, 09	.821052542631, 09
9	-.45856272, -01	-.45856272975402, -01	-.79581870, 09	-.795818718590, 09
10	.18664760, 00	.18664761544688, 00	.77212229, 09	.772122289331, 09
11	-.38809718, -01	-.38809719373731, -01	-.74982404, 09	-.749824039467, 09
12	.15803198, 00	.15803200452627, 00	.72880141, 09	.728801402343, 09
13	-.33640562, -01	-.33640563670387, -01	-.70894600, 09	-.708945995807, 09
14	.13702696, 00	.13702696892367, 00	.69016158, 09	.690161591189, 09
15	-.29686662, -01	-.29686663616401, -01	-.67236245, 09	-.672362427583, 09

The accuracy is at least six significant figures in the ranges mentioned above. This accuracy is enough for the majority of quantum chemistry calculations.

Certification of INTSOLI

Input				Preuss' Result		
n	r	z_a	z_b	K and W Result	Notation	Table No.
1	5	0.5	0.2	s 0.14841691	0.5 0.1 [1a 3b]	23
1	1	4.5	8.0	s 0.35203437	4.5 4.0 [1a 3b]	30
2	1	20	20	s $0.25032133 \times 10^{-1}$	10 10 [2a 3b]	40
1	5	0.5	0.2	$i1$ 0.22058816	0.5 0.1 5[a ⁻¹ 1a 3b]	59
1	1	4.5	8.0	$i1$ 0.96587055	4.5 4.0 1[a ⁻¹ 1a 3b]	66
2	1	20	20	$i1$ $0.58102500 \times 10^{-1}$	10 10 1[a ⁻¹ 2a 3b]	76
1	1	0.5	0.2	$i2$ 0.44818080	0.5 0.5 1[b ⁻¹ 1a 1a]	41
1	5	0.5	0.2	$i2$ 0.97641725	0.5 0.5 5[b ⁻¹ 1a 1a]	45
2	1	20	20	$i2$ 0.99999530	10 10 1[b ⁻¹ 2a 2a]	58
1	1	10	1	$i3$ 0.26217432	0.5 0.5 1[b ⁻¹ 3a 3a]	41
1	1	10	10	$i3$ 0.11093011×10^1	5 5 1[b ⁻¹ 3a 3a]	50
1	1	10	20	$i3$ 0.10300137×10^1	10 10 1[b ⁻¹ 3a 3a]	58