

## ERRATUM

J. Zupan: Computer Program for the Evaluation of Overlap Integrals, *Croat. Chem. Acta* **46** (3) (1974) 199—207.

At the end of the program listing (p. 206) the following functions should be added:

```

FUNCTION A(FN,P)
C      INEGRAL A(FN,P)  WHERE          FN IS ANY REAL NUMBER EXCLUDING
C                                     NEGATIVE INTEGERS
C                                     P IS ANY NONZERO REAL NUMBER
C
      DIMENSION FAK(11)
      DATA FAK/1.0000000000,0.9513507699,0.9181687424,0.8974706963,
X0.8872638175,0.8862269255,0.8935153493,0.9086387329,0.9313837710,
X0.9617658319,1.000000000/
      S=1.
      G=1.
      IT=10.*P+10.
      IF(FN.GE.-0.0001.AND.FN.LE.0.0001)      GO TO 6
      IF(FN) 10,6,20
6      A=EXP(-P)/P
      RETURN
10     NF=ABS(FN)+1
      REL=FN+NF
      GO TO 1
20     NF=IFIX(ABS(FN))
      REL=FN-NF
1      CONTINUE
      NT=IFIX(REL*10.+0.001)+1
      DO 2 J=2,IT
      S=S*P/(REL+J)
      G=G+S
2      CONTINUE
      A=FAK(NT)/(P**(REL+1.))-EXP(-P)*(G)/(REL+1.)
      IF(NF.EQ.0) RETURN
      IF(FN.LT.0.) GO TO 4
      DO 3 J=1,NF
3      A=(EXP(-P)*(REL+J)*A)/P
      RETURN
4      DO 5 J=1,NF
5      A=(P*A-EXP(-P))/(REL-J+1)
      RETURN
      END

FUNCTION B(K,RO)
C      INTEGRAL B(K,RO)  WHERE          K IS NOT NEGATIV INTEGER AND
C                                     RO IS ANY REAL NUMBER
C
      ID=-1
      IF((FLOAT(K)/2-K/2).EQ.0.) ID=1
      IF(ID.EQ.1.AND.RO.EQ.0.) GO TO 3
      R=0.

```