CONTIN (Version 2) Users Manual

(March, 1984)

Part 2

Technical Report EMBL-DA07 (March 1984)

Part 1: Users Manual

Part 2: Output from Test Runs

Users manual for CONTIN — A portable Fortran IV program for the regularized solution of linear algebraic and linear integral equations of the first kind, with options for linear equality and inequality constraints.

Stephen W. Provencher

sp@S-provencher.COM

http://S-provencher.COM

CONTIN - VERSION 2DP (MAR 1984) (PCS-1 PACK) TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

REFERENCES - S.W. PROVENCHER (1982) COMPUT. PHYS. COMMUN., VOL. 27, PAGES 213-227, 229-242.
(1984) EMBL TECHNICAL REPORT DA07 (EUROPEAN MOLECULAR BIOLOGY LABORATORY, HEIDELBERG, F.R. OF GERMANY)

INPUT DATA FOR CHANGES TO COMMON VARIABLES

LAST	0	-1.00000E+00	
GMNMX	1	5.00000E+02	
GMNMX	2	5.00000E+06	
IWT	0	5.00000E+00	
NERFIT	0	0.00000E+00	
NINTT	0	3.00000E+00	
NLINF	0	1.00000E+00	
IFORMY (6F8.6)	0	0.00000E+00	
DOUSNQ	0	1.00000E+00	
IUSER	10	1.00000E+00	
RUSER	15	1.43000E+00	
RUSER	16	4.88000E+02	
RUSER	17	6.00000E+01	
RUSER	18	1.37000E-04	
RUSER	22	-5.00000E-01	
RUSER	10	-1.00000E+00	
END	0	0.00000E+00	
NSTEND	17	5.00000E-06	8.50000E-05
NSTEND	16	9.50000E-05	2.45000E-04
NSTEND	4	2.65000E-04	3.25000E-04

MAR 84 Page 1

MAR 84 Page 2

```
                                         FINAL VALUES OF CONTROL VARIABLES
DFMIN  = 2.00000E+00
SRMIN  = 1.00000E-02
ALPST  = 0.00000E+00 0.00000E+00
GMNMX  = 5.00000E+02 5.00000E+06
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00-1.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.43000E+00 4.88000E+02 6.00000E+01 1.37000E-04 0.00000E+00 1.84118E+05
         4.64422E+06-5.00000E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
IGRID  =           2
IQUAD  =           3
IUNIT  =          -1
IWT    =           5
LINEPG =          60
MIOERR =           5
MPKMOM =           5
MQPITR =          35
NEQ    =           0
NERFIT =           0
NG     =          31
NINTT  =           3
NLINF  =           1
NORDER =           2
ICRIT  =           1           1
IFORMT = (5E15.6)
IFORMW = (5E15.6)
IFORMY = (6F8.6)
IPLFIT =           2           2
IPLRES =           2           2
IPRINT =           4           4
IUSER  =           0           0           0           0           0           0           0           0           0           1
                   0           0           0           0           0           0           0          50           0           0
                   0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0           0           0           0           0
IUSROU =           0           0
LSIGN  =           0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0
MOMNMX =          -1           3
NENDZ  =           2           2
NFLAT  =           0           0           0           0           0           0           0           0
NNSGN  =           0           0
NQPROG =           6           6
NSGN   =           0           0           0           0
DOCHOS =           T
DOMOM  =           T
DOUSIN =           T
DOUSNQ =           T
LAST   =           F
NEWPG1 =           F
NONNEG =           T
ONLY1  =           T
PRWT   =           T
PRY    =           T
SIMULA =           F
LUSER  =           F           F           F           F           F           F           F           F           F           F
                   F           F           F           F           F           F           F           F           F           F
                   F           F           F           F           F           F           F           F           F           F
```

T	Y	T	Y	T	Y	T	Y	T	Y
5.000E-06	6.71565E-01	1.000E-05	6.40401E-01	1.500E-05	6.10346E-01	2.000E-05	5.83154E-01	2.500E-05	5.57062E-01
3.000E-05	5.32512E-01	3.500E-05	5.08776E-01	4.000E-05	4.85827E-01	4.500E-05	4.65630E-01	5.000E-05	4.46515E-01
5.500E-05	4.26056E-01	6.000E-05	4.06806E-01	6.500E-05	3.92105E-01	7.000E-05	3.73747E-01	7.500E-05	3.58781E-01
8.000E-05	3.43080E-01	8.500E-05	3.31479E-01	9.500E-05	3.06780E-01	1.050E-04	2.83829E-01	1.150E-04	2.62155E-01
1.250E-04	2.42237E-01	1.350E-04	2.31004E-01	1.450E-04	2.12779E-01	1.550E-04	1.98950E-01	1.650E-04	1.83082E-01
1.750E-04	1.77724E-01	1.850E-04	1.67245E-01	1.950E-04	1.54842E-01	2.050E-04	1.47347E-01	2.150E-04	1.46741E-01
2.250E-04	1.42520E-01	2.350E-04	1.28402E-01	2.450E-04	1.31195E-01	2.650E-04	1.26795E-01	2.850E-04	1.07968E-01
3.050E-04	1.15698E-01	3.250E-04	1.03947E-01						

PRECIS = 1.86D-16 SRANGE = 1.00E+35 RANGE = 1.00D+35

MAR 84 Page 3

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
5.0000E+02	1.2377D-25	3.25D-04	9.0566D+03	5.00D-06	9.155D-14
6.7968E+02	1.3584D-20	3.25D-04	7.7602D+04	5.00D-06	9.155D-14
9.2392E+02	4.7501D-17	3.25D-04	8.1387D+04	5.00D-06	9.155D-14
1.2559E+03	2.0572D-13	3.25D-04	3.3533D+05	5.00D-06	9.155D-14
1.7073E+03	8.1485D-11	3.25D-04	3.4009D+05	5.00D-06	9.155D-14
2.3208E+03	5.4496D-08	3.25D-04	1.3615D+06	5.00D-06	9.155D-14
3.1548E+03	4.3485D-06	3.25D-04	1.3473D+06	5.00D-06	9.155D-14
4.2885E+03	7.3590D-04	3.25D-04	5.2808D+06	5.00D-06	9.155D-14
5.8296E+03	1.8068D-02	3.25D-04	5.1316D+06	5.00D-06	9.155D-14
7.9245E+03	1.1126D+00	3.25D-04	1.9804D+07	5.00D-06	9.155D-14
1.0772E+04	1.1478D+01	3.25D-04	1.8989D+07	5.00D-06	9.155D-14
1.4643E+04	3.3599D+02	3.25D-04	7.2448D+07	5.00D-06	9.155D-14
1.9905E+04	1.8316D+03	3.25D-04	6.8790D+07	5.00D-06	9.155D-14
2.7058E+04	3.1024D+04	3.25D-04	2.6025D+08	5.00D-06	9.155D-14
3.6782E+04	1.0578D+05	3.25D-04	2.4533D+08	5.00D-06	9.155D-14
5.0000E+04	1.1981D+06	3.25D-04	9.2243D+08	5.00D-06	9.155D-14
6.7968E+04	2.8927D+06	3.25D-04	8.6495D+08	5.00D-06	9.155D-14
9.2393E+04	2.4367D+07	3.25D-04	3.2374D+09	5.00D-06	9.155D-14
1.2559E+05	4.5639D+07	3.25D-04	3.0238D+09	5.00D-06	9.155D-14
1.7073E+05	3.0920D+08	3.25D-04	1.1280D+10	5.00D-06	9.155D-14
2.3208E+05	4.8044D+08	3.25D-04	1.0505D+10	5.00D-06	9.155D-14
3.1548E+05	2.7731D+09	3.25D-04	3.9091D+10	5.00D-06	9.155D-14
4.2885E+05	3.7557D+09	3.25D-04	3.6331D+10	5.00D-06	9.155D-14
5.8296E+05	1.9268D+10	3.25D-04	1.3495D+11	5.00D-06	9.155D-14
7.9245E+05	2.3585D+10	3.25D-04	1.2522D+11	5.00D-06	9.155D-14
1.0772E+06	1.1095D+11	3.25D-04	4.6450D+11	5.00D-06	9.155D-14
1.4643E+06	1.2608D+11	3.25D-04	4.3053D+11	5.00D-06	9.155D-14
1.9905E+06	5.5644D+11	3.25D-04	1.5955D+12	5.00D-06	9.155D-14
2.7059E+06	5.9865D+11	3.25D-04	1.4776D+12	5.00D-06	9.155D-14
3.6782E+06	2.5210D+12	3.25D-04	5.4716D+12	5.00D-06	9.155D-14
5.0000E+06	1.3026D+12	3.25D-04	2.5320D+12	5.00D-06	9.155D-14
NLINF TERMS	1.0000D+00	5.00D-06	1.0000D+00	5.00D-06	2.703D-02

SCALE FACTOR FOR ALPHA = 9.302E+13

1 UNREGULARIZED VARIABLES

SINGULAR VALUES

1.121E+06	3.856E-01	6.655E-03	2.585E-04	1.451E-05	1.175E-06	1.203E-07	1.511E-08	2.436E-09	1.466E-09
8.540E-10	3.602E-10	2.092E-10	1.225E-10	4.340E-11	2.431E-11	1.405E-11	6.253E-12	3.056E-12	2.302E-12
2.100E-12	2.035E-12	5.630E-13	2.804E-13	9.098E-14	4.307E-14	1.285E-14	3.996E-15	9.211E-16	5.740E-16
3.560E-16	2.080E-17								

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION) PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 2.09E-10	1.86E-16	2.83805E-04	2.83805E-04	2.889E-03	3.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA	
0.000E+00	2.9D-29	5.00E+02X	
0.000E+00	5.1D-29	6.80E+02X	
0.000E+00	2.7D-29	9.24E+02X	
0.000E+00	3.8D-29	1.26E+03X	
0.000E+00	2.2D-30	1.71E+03X	
0.000E+00	1.1D-28	2.32E+03X	
0.000E+00	2.4D-28	3.15E+03X	
0.000E+00	1.4D-28	4.29E+03X	
0.000E+00	1.2D-28	5.83E+03X	
0.000E+00	2.3D-28	7.92E+03X	
0.000E+00	4.3D-28	1.08E+04X	
0.000E+00	1.6D-28	1.46E+04X	
0.000E+00	3.1D-28	1.99E+04X	
0.000E+00	1.1D-28	2.71E+04X	
0.000E+00	3.8D-28	3.68E+04X	
0.000E+00	1.3D-28	5.00E+04X	
0.000E+00	1.6D-28	6.80E+04X	
0.000E+00	5.2D-28	9.24E+04X	
0.000E+00	9.4D-28	1.26E+05X	
4.263E-11	3.0D-12	1.71E+05	
1.006E-11	3.2D-12	2.32E+05	.....X.....
0.000E+00	6.4D-28	3.15E+05X	
0.000E+00	4.5D-28	4.29E+05X	
0.000E+00	5.0D-28	5.83E+05X	
0.000E+00	1.0D-27	7.92E+05X	
0.000E+00	6.2D-28	1.08E+06X	
0.000E+00	6.5D-28	1.46E+06X	
0.000E+00	3.1D-28	1.99E+06X	
0.000E+00	2.2D-29	2.71E+06X	
0.000E+00	1.8D-28	3.68E+06X	
0.000E+00	2.9D-28	5.00E+06X	

MAR 84 Page 4

.....X

LINEAR COEFFICIENTS = 8.5963E-02 +- 1.7D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 1.2E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9509 X (10** -11)	2.9E+00			
0	3.4570 X (10** -6)	1.6E+00	1.7720E+05	4.4E+00	0
1	6.1951 X (10** -1)	2.8E-01	1.7921E+05	1.9E+00	1
2	1.1257 X (10** 5)	2.0E+00	1.8171E+05	2.3E+00	2
3	2.0797 X (10** 10)	4.3E+00	1.8475E+05	6.3E+00	3

(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.5018 PUNCOR = 0.1876 0.7394 0.0205 0.8123 0.5932

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION) PRELIMINARY UNWEIGHTED ANALYSIS

	ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
*	5.83E-09	5.20E-15	2.83807E-04	2.83805E-04	2.889E-03	3.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA	
0.000E+00	1.8D-29	5.00E+02	X
0.000E+00	4.5D-29	6.80E+02	X
0.000E+00	1.1D-29	9.24E+02	X
0.000E+00	1.1D-28	1.26E+03	X
0.000E+00	4.7D-30	1.71E+03	X
0.000E+00	1.2D-28	2.32E+03	X
0.000E+00	3.1D-28	3.15E+03	X
0.000E+00	1.7D-28	4.29E+03	X
0.000E+00	2.4D-29	5.83E+03	X
0.000E+00	2.6D-29	7.92E+03	X
0.000E+00	5.8D-29	1.08E+04	X
0.000E+00	6.7D-28	1.46E+04	X
0.000E+00	2.8D-28	1.99E+04	X
0.000E+00	8.3D-28	2.71E+04	X
0.000E+00	1.8D-28	3.68E+04	X
0.000E+00	2.5D-28	5.00E+04	X
0.000E+00	7.5D-28	6.80E+04	X
0.000E+00	6.8D-28	9.24E+04	X
0.000E+00	5.4D-28	1.26E+05	X
4.263E-11	3.0D-12	1.71E+05	X
1.006E-11	3.2D-12	2.32E+05	.....X.....
0.000E+00	1.4D-29	3.15E+05	X
0.000E+00	7.7D-28	4.29E+05	X
0.000E+00	1.2D-28	5.83E+05	X
0.000E+00	1.4D-28	7.92E+05	X
0.000E+00	6.6D-29	1.08E+06	X
0.000E+00	3.6D-28	1.46E+06	X
0.000E+00	4.8D-28	1.99E+06	X
0.000E+00	1.4D-28	2.71E+06	X
0.000E+00	1.9D-28	3.68E+06	X
0.000E+00	1.1D-28	5.00E+06	X

MAR 84 Page 5

LINEAR COEFFICIENTS = 8.5963E-02 +- 1.7D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06 (STD. DEV.)/MEAN = 1.2E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9509 X (10** -11)	2.8E+00			
0	3.4570 X (10** -6)	1.6E+00	1.7720E+05	4.4E+00	0
1	6.1951 X (10** -1)	2.8E-01	1.7921E+05	1.9E+00	1
2	1.1257 X (10** 5)	2.0E+00	1.8171E+05	2.3E+00	2
3	2.0797 X (10** 10)	4.3E+00	1.8475E+05	6.3E+00	3

(FOR ALPHA/S(1) = 5.20E-15) PRUNS = 0.5018 PUNCOR = 0.1876 0.7394 0.0205 0.8123 0.5931

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.63E-07	1.45E-13	2.85652E-04	2.83811E-04	2.889E-03	2.995	0.000	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	1.1D-28	5.00E+02X
0.000E+00	6.9D-29	6.80E+02X
0.000E+00	7.1D-29	9.24E+02X
0.000E+00	2.3D-29	1.26E+03X
0.000E+00	2.4D-29	1.71E+03X
0.000E+00	8.0D-29	2.32E+03X
0.000E+00	2.0D-29	3.15E+03X
0.000E+00	2.9D-28	4.29E+03X
0.000E+00	6.2D-28	5.83E+03X
0.000E+00	2.4D-29	7.92E+03X
0.000E+00	1.7D-29	1.08E+04X
0.000E+00	1.8D-28	1.46E+04X
0.000E+00	7.6D-28	1.99E+04X
0.000E+00	3.2D-28	2.71E+04X
0.000E+00	4.4D-28	3.68E+04X
0.000E+00	1.3D-28	5.00E+04X
0.000E+00	1.6D-28	6.80E+04X
0.000E+00	1.2D-27	9.24E+04X
0.000E+00	1.2D-27	1.26E+05X
4.255E-11	3.0D-12	1.71E+05
1.014E-11	3.2D-12	2.32E+05
0.000E+00	1.4D-27	3.15E+05X
0.000E+00	5.2D-28	4.29E+05X
0.000E+00	6.1D-28	5.83E+05X
0.000E+00	1.3D-28	7.92E+05X
0.000E+00	3.3D-28	1.08E+06X
0.000E+00	5.7D-28	1.46E+06X
0.000E+00	1.1D-28	1.99E+06X
0.000E+00	2.3D-28	2.71E+06X
0.000E+00	1.1D-28	3.68E+06X
0.000E+00	1.2D-28	5.00E+06X

.....X.....

.....X

MAR 84 Page 6

LINEAR COEFFICIENTS = 8.5921E-02 +- 1.7D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 1.2E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9494 X (10** -11)	2.8E+00			
0	3.4555 X (10** -6)	1.6E+00	1.7726E+05	4.4E+00	0
1	6.1952 X (10** -1)	2.8E-01	1.7928E+05	1.9E+00	1
2	1.1263 X (10** 5)	2.0E+00	1.8180E+05	2.3E+00	2
3	2.0821 X (10** 10)	4.3E+00	1.8487E+05	6.3E+00	3

(FOR ALPHA/S(1) = 1.45E-13) PRUNS = 0.5018 PUNCOR = 0.1880 0.7370 0.0204 0.8134 0.5905

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
2.83E-06	2.52E-12	3.35804E-04	3.14394E-04	3.045E-03	3.090	0.683	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	6.8D-30	5.00E+02X
0.000E+00	1.9D-29	6.80E+02X
0.000E+00	3.5D-29	9.24E+02X
0.000E+00	6.4D-29	1.26E+03X
0.000E+00	4.4D-29	1.71E+03X
0.000E+00	8.1D-30	2.32E+03X
0.000E+00	5.2D-29	3.15E+03X
0.000E+00	3.4D-29	4.29E+03X
0.000E+00	4.5D-29	5.83E+03X
0.000E+00	8.9D-29	7.92E+03X
0.000E+00	3.6D-29	1.08E+04X
0.000E+00	1.2D-28	1.46E+04X
0.000E+00	2.4D-29	1.99E+04X
0.000E+00	1.0D-28	2.71E+04X
0.000E+00	9.2D-29	3.68E+04X
0.000E+00	1.5D-28	5.00E+04X
4.444E-12	1.4D-12	6.80E+04
1.269E-11	1.9D-12	9.24E+04
2.100E-11	1.0D-12	1.26E+05
2.294E-11	1.2D-12	1.71E+05
1.407E-11	8.4D-13	2.32E+05
1.937E-12	5.0D-13	3.15E+05
0.000E+00	1.4D-28	4.29E+05X
0.000E+00	1.0D-28	5.83E+05X
0.000E+00	1.6D-28	7.92E+05X
0.000E+00	2.4D-28	1.08E+06X
0.000E+00	2.5D-28	1.46E+06X
0.000E+00	8.6D-29	1.99E+06X
0.000E+00	9.0D-29	2.71E+06X
0.000E+00	4.2D-29	3.68E+06X
0.000E+00	3.3D-29	5.00E+06X

LINEAR COEFFICIENTS = 8.2451E-02 +- 1.9D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 3.4E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.3463 X (10** -11)	4.0E+00			
0	3.6030 X (10** -6)	1.8E+00	1.5356E+05	5.8E+00	0
1	6.2404 X (10** -1)	3.1E-01	1.7320E+05	2.1E+00	1
2	1.2051 X (10** 5)	2.2E+00	1.9312E+05	2.6E+00	2
3	2.5652 X (10** 10)	5.0E+00	2.1286E+05	7.2E+00	3

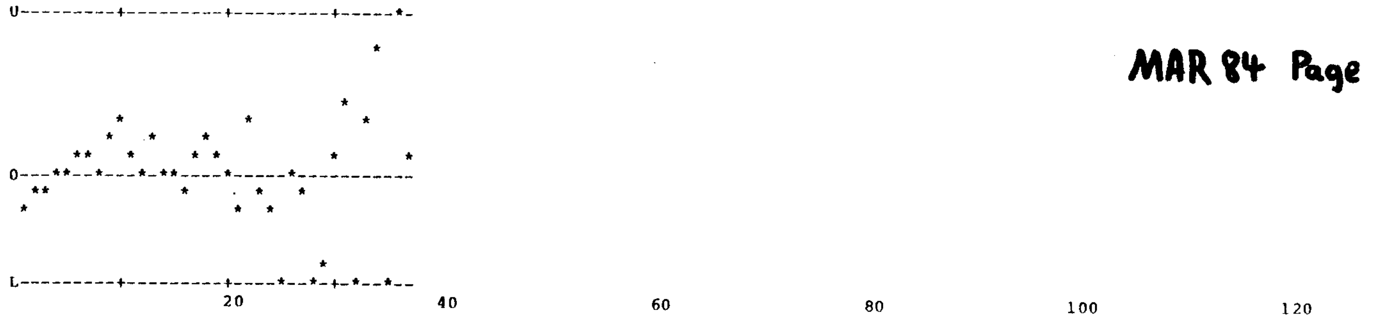
(FOR ALPHA/S(1) = 2.52E-12) PRUNS = 0.1597 PUNCOR = 0.5188 0.9485 0.0103 0.6535 0.6671

MAR 84 Page 12

CONTIN 2DP (MAR 84) (PCS-1)   TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)   CHOSEN SOLUTION

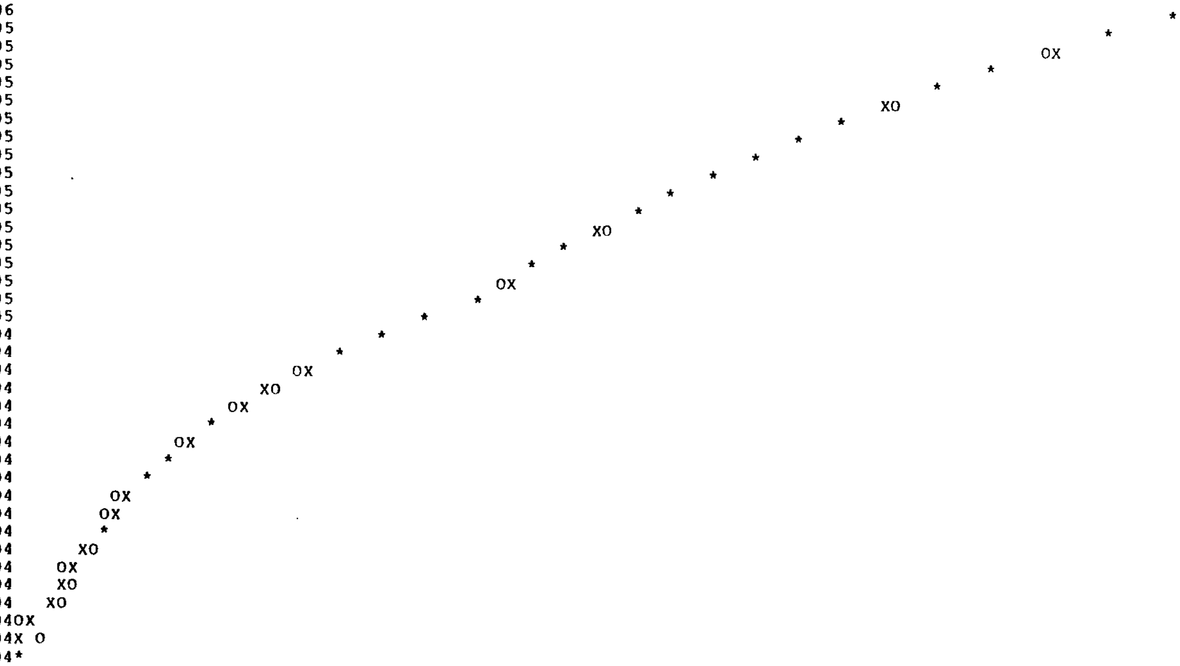
WEIGHTED RESIDUALS (ALPHA/S(1)= 2.52E-12) MAX=U= 8.1E-03 MIN=L=-5.6E-03 (PRUNS= 0.1597) PUNCOR= 0.5188 0.9485 0.0103 0.6535 0.6671

MAR 84 Page 16



PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
6.731E-01	5.00E-06
6.416E-01	1.00E-05
6.118E-01	1.50E-05
5.836E-01	2.00E-05
5.570E-01	2.50E-05
5.318E-01	3.00E-05
5.080E-01	3.50E-05
4.855E-01	4.00E-05
4.642E-01	4.50E-05
4.440E-01	5.00E-05
4.250E-01	5.50E-05
4.070E-01	6.00E-05
3.899E-01	6.50E-05
3.738E-01	7.00E-05
3.585E-01	7.50E-05
3.441E-01	8.00E-05
3.304E-01	8.50E-05
3.053E-01	9.50E-05
2.827E-01	1.05E-04
2.625E-01	1.15E-04
2.444E-01	1.25E-04
2.281E-01	1.35E-04
2.135E-01	1.45E-04
2.004E-01	1.55E-04
1.887E-01	1.65E-04
1.781E-01	1.75E-04
1.686E-01	1.85E-04
1.601E-01	1.95E-04
1.524E-01	2.05E-04
1.455E-01	2.15E-04
1.393E-01	2.25E-04
1.338E-01	2.35E-04
1.287E-01	2.45E-04
1.202E-01	2.65E-04
1.132E-01	2.85E-04
1.075E-01	3.05E-04
1.030E-01	3.25E-04



ERRFIT = 0.00E+00

SQUARE ROOTS OF LEAST SQUARES WEIGHTS

1.1168E+00	1.0800E+00	1.0437E+00	1.0081E+00	9.7316E-01	9.3904E-01	9.0578E-01	8.7344E-01	8.4205E-01	8.1164E-01
7.8226E-01	7.5389E-01	7.2657E-01	7.0027E-01	6.7500E-01	6.5075E-01	6.2750E-01	5.8392E-01	5.4408E-01	5.0777E-01
4.7474E-01	4.4476E-01	4.1759E-01	3.9300E-01	3.7076E-01	3.5067E-01	3.3252E-01	3.1614E-01	3.0136E-01	2.8803E-01
2.7600E-01	2.6516E-01	2.5538E-01	2.3861E-01	2.2497E-01	2.1387E-01	2.0483E-01			

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
5.0000E+02	2.5351D-26	3.25D-04	1.0114D+04	5.00D-06	1.422D-13
6.7968E+02	2.7823D-21	3.25D-04	8.6666D+04	5.00D-06	1.422D-13
9.2392E+02	9.7296D-18	3.25D-04	9.0893D+04	5.00D-06	1.422D-13
1.2559E+03	4.2137D-14	3.25D-04	3.7449D+05	5.00D-06	1.422D-13
1.7073E+03	1.6690D-11	3.25D-04	3.7982D+05	5.00D-06	1.422D-13
2.3208E+03	1.1162D-08	3.25D-04	1.5206D+06	5.00D-06	1.422D-13
3.1548E+03	8.9068D-07	3.25D-04	1.5046D+06	5.00D-06	1.422D-13
4.2885E+03	1.5073D-04	3.25D-04	5.8976D+06	5.00D-06	1.422D-13
5.8296E+03	3.7008D-03	3.25D-04	5.7310D+06	5.00D-06	1.422D-13
7.9245E+03	2.2789D-01	3.25D-04	2.2117D+07	5.00D-06	1.422D-13
1.0772E+04	2.3510D+00	3.25D-04	2.1207D+07	5.00D-06	1.422D-13
1.4643E+04	6.8820D+01	3.25D-04	8.0910D+07	5.00D-06	1.422D-13
1.9905E+04	3.7516D+02	3.25D-04	7.6824D+07	5.00D-06	1.422D-13
2.7058E+04	6.3546D+03	3.25D-04	2.9065D+08	5.00D-06	1.422D-13
3.6782E+04	2.1667D+04	3.25D-04	2.7399D+08	5.00D-06	1.422D-13
5.0000E+04	2.4541D+05	3.25D-04	1.0302D+09	5.00D-06	1.422D-13
6.7968E+04	5.9251D+05	3.25D-04	9.6597D+08	5.00D-06	1.422D-13
9.2393E+04	4.9911D+06	3.25D-04	3.6155D+09	5.00D-06	1.422D-13
1.2559E+05	9.3480D+06	3.25D-04	3.3769D+09	5.00D-06	1.422D-13
1.7073E+05	6.3333D+07	3.25D-04	1.2597D+10	5.00D-06	1.422D-13
2.3208E+05	9.8408D+07	3.25D-04	1.1732D+10	5.00D-06	1.422D-13
3.1548E+05	5.6801D+08	3.25D-04	4.3657D+10	5.00D-06	1.422D-13
4.2885E+05	7.6926D+08	3.25D-04	4.0574D+10	5.00D-06	1.422D-13
5.8296E+05	3.9465D+09	3.25D-04	1.5071D+11	5.00D-06	1.422D-13
7.9245E+05	4.8309D+09	3.25D-04	1.3985D+11	5.00D-06	1.422D-13
1.0772E+06	2.2725D+10	3.25D-04	5.1875D+11	5.00D-06	1.422D-13
1.4643E+06	2.5824D+10	3.25D-04	4.8082D+11	5.00D-06	1.422D-13
1.9905E+06	1.1397D+11	3.25D-04	1.7818D+12	5.00D-06	1.422D-13
2.7059E+06	1.2262D+11	3.25D-04	1.6501D+12	5.00D-06	1.422D-13
3.6782E+06	5.1638D+11	3.25D-04	6.1107D+12	5.00D-06	1.422D-13
5.0000E+06	2.6682D+11	3.25D-04	2.8278D+12	5.00D-06	1.422D-13
NLINF TERMS	2.0483D-01	3.25D-04	1.1168D+00	5.00D-06	4.648D-02

MAR 84 Page 17

SCALE FACTOR FOR ALPHA = 5.990E+13

1 UNREGULARIZED VARIABLES

SINGULAR VALUES

1.246E+06	2.723E-01	4.915E-03	1.845E-04	1.125E-05	9.320E-07	9.612E-08	1.213E-08	2.137E-09	1.346E-09
9.343E-10	2.870E-10	2.296E-10	1.325E-10	4.528E-11	2.608E-11	1.294E-11	6.356E-12	2.732E-12	2.497E-12
1.800E-12	9.611E-13	1.926E-13	1.438E-13	1.390E-13	2.977E-14	5.211E-15	4.527E-15	1.013E-15	3.451E-16
3.199E-17	1.969E-18								

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

	ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
*	2.32E-10	1.86E-16	2.91111E-05	2.91111E-05	9.253E-04	3.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA	
0.000E+00	1.2D-29	5.00E+02	X
0.000E+00	2.9D-29	6.80E+02	X
0.000E+00	2.8D-30	9.24E+02	X
0.000E+00	8.0D-29	1.26E+03	X
0.000E+00	8.9D-29	1.71E+03	X
0.000E+00	6.4D-29	2.32E+03	X
0.000E+00	1.3D-28	3.15E+03	X
0.000E+00	1.5D-28	4.29E+03	X
0.000E+00	1.0D-28	5.83E+03	X
0.000E+00	2.0D-28	7.92E+03	X
0.000E+00	2.3D-28	1.08E+04	X
0.000E+00	5.9D-29	1.46E+04	X
0.000E+00	3.1D-28	1.99E+04	X
0.000E+00	1.6D-29	2.71E+04	X
0.000E+00	1.2D-28	3.68E+04	X
0.000E+00	3.7D-28	5.00E+04	X
0.000E+00	5.3D-29	6.80E+04	X
0.000E+00	2.7D-28	9.24E+04	X
0.000E+00	5.8D-30	1.26E+05	X
3.874E-11	1.9D-12	1.71E+05	X
1.438E-11	2.1D-12	2.32E+05	......X.....
0.000E+00	7.6D-29	3.15E+05	X
0.000E+00	3.9D-28	4.29E+05	X
0.000E+00	7.4D-28	5.83E+05	X
0.000E+00	7.9D-28	7.92E+05	X
0.000E+00	2.6D-29	1.08E+06	X
0.000E+00	8.9D-29	1.46E+06	X
0.000E+00	2.8D-29	1.99E+06	X
0.000E+00	1.1D-28	2.71E+06	X
0.000E+00	9.3D-29	3.68E+06	X
0.000E+00	3.3D-29	5.00E+06	X

MAR 84 Page 18

LINEAR COEFFICIENTS = 8.3409E-02 +- 1.7D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06 (STD. DEV.)/MEAN = 1.3E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.8802 X (10** -11)	1.7E+00			
0	3.3907 X (10** -6)	8.8E-01	1.8033E+05	2.6E+00	0
1	6.2080 X (10** -1)	2.4E-01	1.8309E+05	1.1E+00	1
2	1.1571 X (10** 5)	1.4E+00	1.8640E+05	1.6E+00	2
3	2.2013 X (10** 10)	2.8E+00	1.9024E+05	4.2E+00	3

(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.5018 PUNCOR = 0.6577 0.4703 0.2459 0.2317 0.6489

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

	ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
*	5.15E-09	4.13E-15	2.91117E-05	2.91111E-05	9.253E-04	3.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	1.7D-29	5.00E+02X
0.000E+00	2.8D-29	6.80E+02X
0.000E+00	1.1D-29	9.24E+02X
0.000E+00	2.3D-29	1.26E+03X
0.000E+00	2.4D-29	1.71E+03X
0.000E+00	1.3D-29	2.32E+03X
0.000E+00	1.2D-28	3.15E+03X
0.000E+00	2.1D-28	4.29E+03X
0.000E+00	1.2D-28	5.83E+03X
0.000E+00	2.1D-28	7.92E+03X
0.000E+00	7.3D-29	1.08E+04X
0.000E+00	2.1D-29	1.46E+04X
0.000E+00	2.1D-28	1.99E+04X
0.000E+00	3.1D-29	2.71E+04X
0.000E+00	6.6D-30	3.68E+04X
0.000E+00	4.3D-29	5.00E+04X
0.000E+00	2.1D-28	6.80E+04X
0.000E+00	1.4D-28	9.24E+04X
0.000E+00	1.9D-28	1.26E+05X
3.874E-11	1.9D-12	1.71E+05
1.438E-11	2.1D-12	2.32E+05
0.000E+00	7.1D-28	3.15E+05X
0.000E+00	1.6D-28	4.29E+05X
0.000E+00	5.0D-28	5.83E+05X
0.000E+00	5.5D-28	7.92E+05X
0.000E+00	9.1D-28	1.08E+06X
0.000E+00	9.5D-29	1.46E+06X
0.000E+00	4.2D-28	1.99E+06X
0.000E+00	9.3D-29	2.71E+06X
0.000E+00	3.0D-28	3.68E+06X
0.000E+00	1.8D-29	5.00E+06X

MAR 84 Page 19

LINEAR COEFFICIENTS = 8.3409E-02 +- 1.7D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 1.3E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.8802 X (10** -11)	1.7E+00			
0	3.3907 X (10** -6)	8.8E-01	1.8033E+05	2.6E+00	0
1	6.2080 X (10** -1)	2.4E-01	1.8309E+05	1.1E+00	1
2	1.1571 X (10** 5)	1.4E+00	1.8640E+05	1.6E+00	2
3	2.2013 X (10** 10)	2.8E+00	1.9024E+05	4.2E+00	3

(FOR ALPHA/S(1) = 4.13E-15) PRUNS = 0.5018 PUNCOR = 0.6577 0.4703 0.2459 0.2317 0.6489

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.14E-07	9.16E-14	2.93815E-05	2.91117E-05	9.253E-04	2.996	0.000	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	2.5D-30	5.00E+02X
0.000E+00	1.9D-29	6.80E+02X
0.000E+00	3.3D-29	9.24E+02X
0.000E+00	1.3D-29	1.26E+03X
0.000E+00	1.5D-28	1.71E+03X
0.000E+00	2.5D-30	2.32E+03X
0.000E+00	9.8D-29	3.15E+03X
0.000E+00	6.6D-29	4.29E+03X
0.000E+00	1.3D-28	5.83E+03X
0.000E+00	2.1D-28	7.92E+03X
0.000E+00	3.6D-28	1.08E+04X
0.000E+00	2.3D-28	1.46E+04X
0.000E+00	2.7D-28	1.99E+04X
0.000E+00	1.9D-28	2.71E+04X
0.000E+00	2.3D-28	3.68E+04X
0.000E+00	4.0D-28	5.00E+04X
0.000E+00	4.9D-28	6.80E+04X
0.000E+00	5.6D-29	9.24E+04X
0.000E+00	1.9D-28	1.26E+05X
3.869E-11	1.8D-12	1.71E+05
1.444E-11	2.1D-12	2.32E+05
0.000E+00	2.6D-28	3.15E+05X
0.000E+00	4.3D-28	4.29E+05X
0.000E+00	2.7D-28	5.83E+05X
0.000E+00	8.6D-29	7.92E+05X
0.000E+00	1.2D-28	1.08E+06X
0.000E+00	8.2D-29	1.46E+06X
0.000E+00	3.0D-28	1.99E+06X
0.000E+00	2.4D-28	2.71E+06X
0.000E+00	2.0D-28	3.68E+06X
0.000E+00	8.7D-29	5.00E+06X

MAR 84 Page 20

.....X.....

....X

LINEAR COEFFICIENTS = 8.3370E-02 +- 1.7D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 1.3E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.8794 X (10** -11)	1.7E+00			
0	3.3899 X (10** -6)	8.8E-01	1.8037E+05	2.6E+00	0
1	6.2082 X (10** -1)	2.4E-01	1.8314E+05	1.1E+00	1
2	1.1576 X (10** 5)	1.4E+00	1.8645E+05	1.6E+00	2
3	2.2029 X (10** 10)	2.7E+00	1.9030E+05	4.1E+00	3

(FOR ALPHA/S(1) = 9.16E-14) PRUNS = 0.5018

PUNCOR = 0.6572 0.4685 0.2455 0.2314 0.6486

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
2.53E-06	2.03E-12	3.84872E-05	3.50885E-05	1.018E-03	3.131	0.908	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	1.6D-30	5.00E+02X
0.000E+00	3.1D-29	6.80E+02X
0.000E+00	3.3D-29	9.24E+02X
0.000E+00	2.8D-29	1.26E+03X
0.000E+00	4.0D-29	1.71E+03X
0.000E+00	2.2D-29	2.32E+03X
0.000E+00	3.4D-29	3.15E+03X
0.000E+00	3.0D-29	4.29E+03X
0.000E+00	7.5D-29	5.83E+03X
0.000E+00	6.5D-29	7.92E+03X
0.000E+00	4.4D-29	1.08E+04X
0.000E+00	7.2D-29	1.46E+04X
0.000E+00	2.9D-28	1.99E+04X
0.000E+00	2.6D-28	2.71E+04X
0.000E+00	2.7D-28	3.68E+04X
1.757E-12	1.0D-12	5.00E+04
6.921E-12	1.5D-12	6.80E+04
1.375E-11	1.1D-12	9.24E+04
1.915E-11	5.6D-13	1.26E+05
1.947E-11	9.5D-13	1.71E+05
1.259E-11	5.0D-13	2.32E+05
3.399E-12	3.6D-13	3.15E+05
0.000E+00	2.4D-28	4.29E+05X
0.000E+00	3.5D-29	5.83E+05X
0.000E+00	7.0D-29	7.92E+05X
0.000E+00	5.7D-29	1.08E+06X
0.000E+00	1.1D-28	1.46E+06X
0.000E+00	2.5D-29	1.99E+06X
0.000E+00	1.1D-28	2.71E+06X
0.000E+00	1.2D-29	3.68E+06X
0.000E+00	1.9D-29	5.00E+06X

LINEAR COEFFICIENTS = 7.7108E-02 +- 1.8D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 3.9E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.3620 X (10** -11)	3.6E+00			
0	3.5420 X (10** -6)	1.2E+00	1.4996E+05	4.8E+00	0
1	6.2778 X (10** -1)	2.7E-01	1.7724E+05	1.5E+00	1
2	1.2830 X (10** 5)	1.6E+00	2.0437E+05	1.9E+00	2
3	2.9450 X (10** 10)	3.2E+00	2.2954E+05	4.8E+00	3

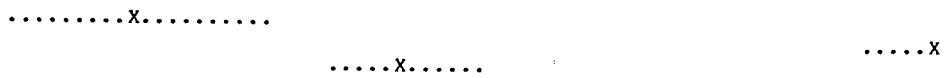
(FOR ALPHA/S(1) = 2.03E-12) PRUNS = 0.1671 PUNCOR = 0.5745 0.8722 0.0873 0.1388 0.8420

MAR 84 Page 21

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
2.77E-07	2.22E-13	3.00056E-05	2.95693E-05	9.328E-04	3.020	0.090	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	7.3D-30	5.00E+02X
0.000E+00	3.3D-29	6.80E+02X
0.000E+00	4.6D-29	9.24E+02X
0.000E+00	2.7D-29	1.26E+03X
0.000E+00	1.1D-28	1.71E+03X
0.000E+00	6.6D-29	2.32E+03X
0.000E+00	6.2D-29	3.15E+03X
0.000E+00	1.0D-28	4.29E+03X
0.000E+00	8.9D-29	5.83E+03X
0.000E+00	1.3D-28	7.92E+03X
0.000E+00	1.7D-28	1.08E+04X
0.000E+00	6.0D-29	1.46E+04X
0.000E+00	2.4D-28	1.99E+04X
0.000E+00	3.0D-28	2.71E+04X
0.000E+00	4.4D-28	3.68E+04X
0.000E+00	2.4D-28	5.00E+04X
0.000E+00	4.1D-28	6.80E+04X
0.000E+00	8.9D-28	9.24E+04X
1.245E-11	3.0D-12	1.26E+05
3.141E-11	1.6D-12	1.71E+05
1.874E-11	1.7D-12	2.32E+05
0.000E+00	6.6D-28	3.15E+05X
0.000E+00	8.2D-28	4.29E+05X
0.000E+00	6.2D-28	5.83E+05X
0.000E+00	4.0D-28	7.92E+05X
0.000E+00	6.1D-28	1.08E+06X
0.000E+00	6.2D-28	1.46E+06X
0.000E+00	4.2D-28	1.99E+06X
0.000E+00	2.3D-28	2.71E+06X
0.000E+00	2.0D-28	3.68E+06X
0.000E+00	1.0D-28	5.00E+06X



LINEAR COEFFICIENTS = 8.2731E-02 +- 1.6D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 1.8E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9240 X (10** -11)	2.1E+00			
0	3.4052 X (10** -6)	9.4E-01	1.7698E+05	3.0E+00	0
1	6.2154 X (10** -1)	2.3E-01	1.8253E+05	1.2E+00	1
2	1.1697 X (10** 5)	1.3E+00	1.8820E+05	1.5E+00	2
3	2.2685 X (10** 10)	2.3E+00	1.9393E+05	3.6E+00	3

(FOR ALPHA/S(1) = 2.22E-13) PRUNS = 0.5018 PUNCOR = 0.7268 0.5195 0.2245 0.2214 0.6632

MAR 84 Page 24

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
6.71E-07	5.39E-13	3.17817E-05	2.98263E-05	9.407E-04	3.298	0.159	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	2.0D-29	5.00E+02X
0.000E+00	6.0D-29	6.80E+02X
0.000E+00	7.8D-29	9.24E+02X
0.000E+00	1.2D-28	1.26E+03X
0.000E+00	3.1D-28	1.71E+03X
0.000E+00	4.0D-28	2.32E+03X
0.000E+00	4.2D-28	3.15E+03X
0.000E+00	4.9D-28	4.29E+03X
0.000E+00	3.5D-28	5.83E+03X
0.000E+00	7.1D-28	7.92E+03X
0.000E+00	4.5D-28	1.08E+04X
0.000E+00	4.5D-28	1.46E+04X
0.000E+00	7.6D-29	1.99E+04X
0.000E+00	1.9D-28	2.71E+04X
0.000E+00	4.5D-29	3.68E+04X
0.000E+00	2.3D-28	5.00E+04X
0.000E+00	3.8D-28	6.80E+04X
7.458E-13	4.1D-12	9.24E+04..X.....
1.594E-11	2.0D-12	1.26E+05
2.881E-11	2.6D-12	1.71E+05
2.012E-11	2.5D-12	2.32E+05
5.441E-14	9.9D-13	3.15E+05X...
0.000E+00	8.1D-29	4.29E+05X
0.000E+00	3.1D-28	5.83E+05X
0.000E+00	1.6D-28	7.92E+05X
0.000E+00	2.9D-28	1.08E+06X
0.000E+00	3.9D-29	1.46E+06X
0.000E+00	2.0D-28	1.99E+06X
0.000E+00	1.4D-28	2.71E+06X
0.000E+00	5.1D-29	3.68E+06X
0.000E+00	1.9D-29	5.00E+06X

MAR 84 Page 25

.....X.....

.....X.....

.....X

LINEAR COEFFICIENTS = 8.2437E-02 +- 2.2D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 2.0E-01

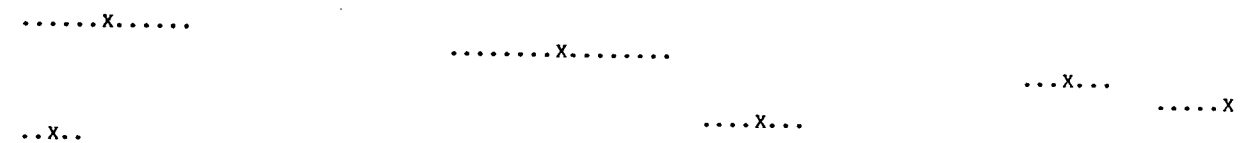
J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9502 X (10** -11)	5.0E+00			
0	3.4143 X (10** -6)	1.3E+00	1.7507E+05	6.3E+00	0
1	6.2188 X (10** -1)	3.5E-01	1.8214E+05	1.6E+00	1
2	1.1758 X (10** 5)	2.9E+00	1.8907E+05	3.2E+00	2
3	2.3023 X (10** 10)	8.3E+00	1.9581E+05	1.1E+01	3

(FOR ALPHA/S(1) = 5.39E-13) PRUNS = 0.5018 PUNCOR = 0.7662 0.5505 0.2141 0.2163 0.6721

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.63E-06	1.31E-12	3.57887E-05	3.31443E-05	9.893E-04	3.137	0.785	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	1.1D-29	5.00E+02X
0.000E+00	4.0D-29	6.80E+02X
0.000E+00	3.0D-30	9.24E+02X
0.000E+00	1.3D-29	1.26E+03X
0.000E+00	7.8D-29	1.71E+03X
0.000E+00	4.5D-29	2.32E+03X
0.000E+00	7.0D-29	3.15E+03X
0.000E+00	4.7D-29	4.29E+03X
0.000E+00	8.6D-29	5.83E+03X
0.000E+00	3.0D-29	7.92E+03X
0.000E+00	9.8D-29	1.08E+04X
0.000E+00	1.5D-28	1.46E+04X
0.000E+00	9.9D-29	1.99E+04X
0.000E+00	9.7D-29	2.71E+04X
0.000E+00	6.2D-29	3.68E+04X
0.000E+00	6.9D-29	5.00E+04X
3.437E-12	1.4D-12	6.80E+04
1.092E-11	1.7D-12	9.24E+04
1.936E-11	6.2D-13	1.26E+05
2.207E-11	1.2D-12	1.71E+05
1.417E-11	8.4D-13	2.32E+05
2.517E-12	4.6D-13	3.15E+05
0.000E+00	1.2D-28	4.29E+05X
0.000E+00	3.2D-29	5.83E+05X
0.000E+00	1.4D-28	7.92E+05X
0.000E+00	1.6D-28	1.08E+06X
0.000E+00	4.0D-29	1.46E+06X
0.000E+00	1.7D-28	1.99E+06X
0.000E+00	4.9D-29	2.71E+06X
0.000E+00	7.7D-30	3.68E+06X
0.000E+00	1.9D-29	5.00E+06X



MAR 84 Page 26

LINEAR COEFFICIENTS = 7.8725E-02 +- 1.9D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 3.4E-01

(FOR ALPHA/S(1) = 1.31E-12) PRUNS = 0.3709

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.2100 X (10** -11)	3.1E+00			
0	3.4989 X (10** -6)	1.1E+00	1.5832E+05	4.1E+00	0
1	6.2598 X (10** -1)	2.8E-01	1.7891E+05	1.4E+00	1
2	1.2516 X (10** 5)	1.8E+00	1.9994E+05	2.0E+00	2
3	2.7622 X (10** 10)	3.9E+00	2.2070E+05	5.7E+00	3

PUNCOR = 0.7808 0.9260 0.1196 0.1623 0.7794

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
3.94E-06	3.16E-12	4.19747E-05	3.73014E-05	1.049E-03	3.091	0.964	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	6.2D-30	5.00E+02X
0.000E+00	3.0D-29	6.80E+02X
0.000E+00	1.9D-29	9.24E+02X
0.000E+00	2.2D-29	1.26E+03X
0.000E+00	7.4D-30	1.71E+03X
0.000E+00	4.5D-29	2.32E+03X
0.000E+00	5.2D-30	3.15E+03X
0.000E+00	8.9D-30	4.29E+03X
0.000E+00	1.7D-29	5.83E+03X
0.000E+00	3.5D-29	7.92E+03X
0.000E+00	5.0D-29	1.08E+04X
0.000E+00	6.9D-29	1.46E+04X
0.000E+00	2.0D-28	1.99E+04X
0.000E+00	2.3D-28	2.71E+04X
1.496E-12	5.8D-13	3.68E+04
4.923E-12	1.1D-12	5.00E+04
1.003E-11	1.1D-12	6.80E+04
1.518E-11	7.2D-13	9.24E+04
1.826E-11	5.4D-13	1.26E+05
1.736E-11	6.2D-13	1.71E+05
1.159E-11	2.8D-13	2.32E+05
4.116E-12	2.7D-13	3.15E+05
0.000E+00	9.6D-29	4.29E+05X
0.000E+00	7.5D-29	5.83E+05X
0.000E+00	1.4D-28	7.92E+05X
0.000E+00	4.1D-29	1.08E+06X
0.000E+00	1.1D-29	1.46E+06X
0.000E+00	8.9D-30	1.99E+06X
0.000E+00	5.9D-30	2.71E+06X
0.000E+00	3.2D-29	3.68E+06X
0.000E+00	1.9D-29	5.00E+06X

MAR 84 Page 27

LINEAR COEFFICIENTS = 7.5605E-02 +- 1.8D-03

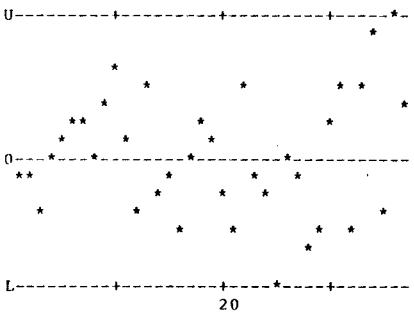
PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 4.3E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.5486 X (10** -11)	3.5E+00			
0	3.5900 X (10** -6)	1.2E+00	1.4086E+05	4.7E+00	0
1	6.2948 X (10** -1)	2.6E-01	1.7534E+05	1.5E+00	1
2	1.3113 X (10** 5)	1.4E+00	2.0832E+05	1.7E+00	2
3	3.1049 X (10** 10)	2.6E+00	2.3678E+05	4.0E+00	3

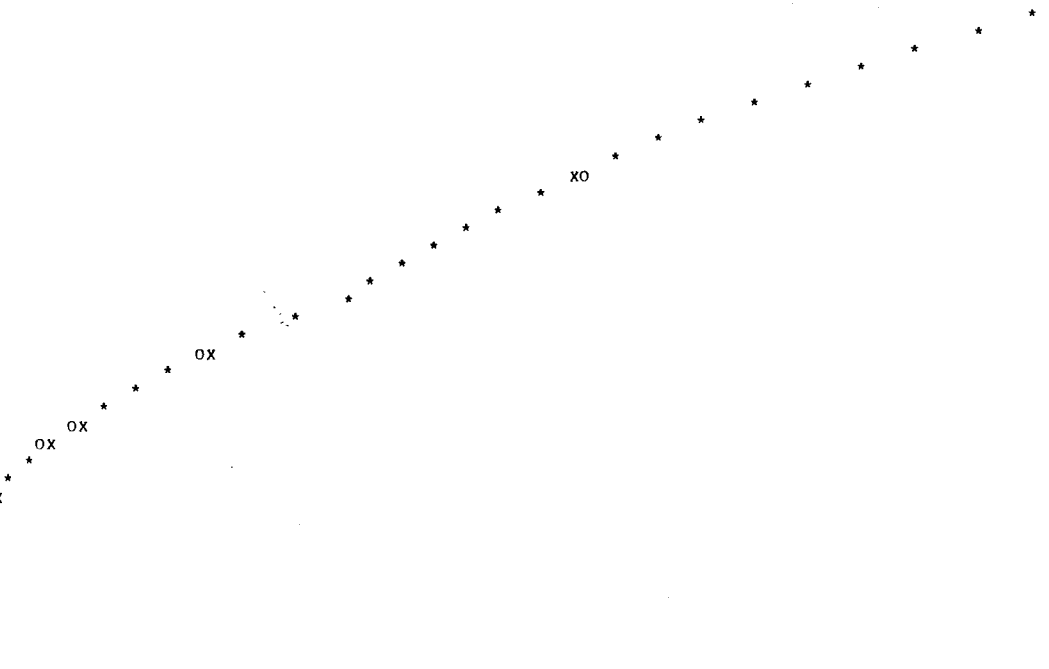
(FOR ALPHA/S(1) = 3.16E-12) PRUNS = 0.0479 PUNCOR = 0.3958 0.6727 0.0625 0.1177 0.9101

WEIGHTED RESIDUALS (ALPHA/S(1)= 1.31E-12) MAX=U= 2.2E-03 MIN=L=-2.0E-03 (PRUNS= 0.3709) PUNCOR= 0.7808 0.9260 0.1196 0.1623 0.7794



PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
6.718E-01	5.00E-06
6.406E-01	1.00E-05
6.111E-01	1.50E-05
5.832E-01	2.00E-05
5.569E-01	2.50E-05
5.319E-01	3.00E-05
5.083E-01	3.50E-05
4.859E-01	4.00E-05
4.647E-01	4.50E-05
4.447E-01	5.00E-05
4.257E-01	5.50E-05
4.078E-01	6.00E-05
3.908E-01	6.50E-05
3.747E-01	7.00E-05
3.594E-01	7.50E-05
3.450E-01	8.00E-05
3.313E-01	8.50E-05
3.060E-01	9.50E-05
2.834E-01	1.05E-04
2.630E-01	1.15E-04
2.448E-01	1.25E-04
2.284E-01	1.35E-04
2.136E-01	1.45E-04
2.003E-01	1.55E-04
1.884E-01	1.65E-04
1.777E-01	1.75E-04
1.680E-01	1.85E-04
1.593E-01	1.95E-04
1.515E-01	2.05E-04
1.444E-01	2.15E-04
1.381E-01	2.25E-04
1.324E-01	2.35E-04
1.272E-01	2.45E-04
1.184E-01	2.65E-04
1.112E-01	2.85E-04
1.053E-01	3.05E-04
1.005E-01	3.25E-04

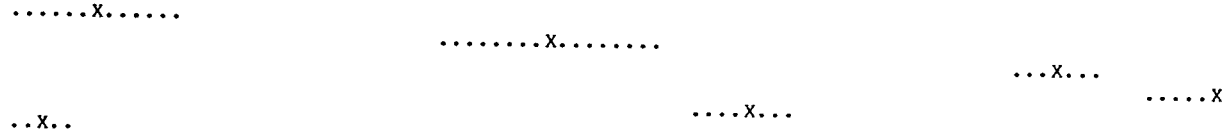


CONTIN VERSION 2DP (MAR 1984) (PCS-1 PACKAGE) ++++++++++++++++++++++++++++++++ CHOSEN SOLUTION ++++++++++++++++++++++++++++++++

TEST DATA SET 1 (MOLECULAR WEIGHT DISTRIBUTION)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.63E-06	1.31E-12	3.57887E-05	3.31443E-05	9.893E-04	3.137	0.785	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	3.1D-29	5.00E+02X
0.000E+00	2.6D-29	6.80E+02X
0.000E+00	2.2D-29	9.24E+02X
0.000E+00	2.2D-29	1.26E+03X
0.000E+00	1.9D-29	1.71E+03X
0.000E+00	7.7D-29	2.32E+03X
0.000E+00	2.4D-29	3.15E+03X
0.000E+00	2.7D-29	4.29E+03X
0.000E+00	1.3D-28	5.83E+03X
0.000E+00	5.9D-29	7.92E+03X
0.000E+00	7.8D-29	1.08E+04X
0.000E+00	1.3D-28	1.46E+04X
0.000E+00	1.1D-28	1.99E+04X
0.000E+00	2.6D-28	2.71E+04X
0.000E+00	2.2D-28	3.68E+04X
0.000E+00	8.9D-29	5.00E+04X
3.437E-12	1.4D-12	6.80E+04
1.092E-11	1.7D-12	9.24E+04
1.936E-11	6.2D-13	1.26E+05
2.207E-11	1.2D-12	1.71E+05
1.417E-11	8.4D-13	2.32E+05
2.517E-12	4.6D-13	3.15E+05
0.000E+00	2.1D-28	4.29E+05X
0.000E+00	2.4D-28	5.83E+05X
0.000E+00	1.1D-28	7.92E+05X
0.000E+00	2.7D-28	1.08E+06X
0.000E+00	1.9D-28	1.46E+06X
0.000E+00	1.3D-28	1.99E+06X
0.000E+00	1.8D-28	2.71E+06X
0.000E+00	4.7D-29	3.68E+06X
0.000E+00	5.5D-29	5.00E+06X



MAR 84 Page 31

LINEAR COEFFICIENTS = 7.8725E-02 +- 1.9D-03

PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 3.4E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.2100 X (10** -11)	3.1E+00			
0	3.4989 X (10** -6)	1.1E+00	1.5832E+05	4.1E+00	0
1	6.2598 X (10** -1)	2.8E-01	1.7891E+05	1.4E+00	1
2	1.2516 X (10** 5)	1.8E+00	1.9994E+05	2.0E+00	2
3	2.7622 X (10** 10)	3.9E+00	2.2070E+05	5.7E+00	3

FINAL VALUES OF CONTROL VARIABLES

```
DFMIN  = 2.00000E+00
SRMIN  = 1.00000E-02
ALPST  = 0.00000E+00 0.00000E+00
GMNMX  = 1.00000E-06 1.00000E-04
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 2.00000E-04 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00-1.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.43000E+00 4.88000E+02 6.00000E+01 2.98000E+02 8.93700E-01 1.84118E+05
         8.27835E-03-1.00000E+00 0.00000E+00 0.00000E+00 1.50000E-05 3.50000E-01 5.00000E-06 3.50000E-01 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         3.50000E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00
         1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00
         1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00
         1.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
IGRID  =           2
IQUAD  =           3
IUNIT  =          -1
IWT    =           5
LINEPG =          60
MIOERR =           5
MPKMOM =           5
MQPITR =          35
NEQ    =           0
NERFIT =           0
NG     =          31
NINTT  =           1
NLINF  =           1
NORDER =           2
ICRIT  =           1           1
IFORMT = (5E15.6)
IFORMW = (5E15.6)
IFORMY = (6F8.6)
IPLFIT =           2           2
IPLRES =           2           2
IPRINT =           4           4
IUSER  =           0           0       30171           0           0           0           0           0           0           3
                   2           0           0           0           0           0           0          50           0           0
                   0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0           0           0           0           0
IUSROU =           0           0
LSIGN  =           0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0
MQMNMX =          -3           3
NENDZ  =           2           2
NFLAT  =           0           0           0           0           0           0           0           0
NNSGN  =           0           0
NQPROG =           6           6
NSGN   =           0           0           0           0
DOCHOS =           T
DOMOM  =           T
DOUSIN =           T
DOUSNQ =           T
LAST   =           T
NEWPG1 =           T
NONNEG =           T
ONLY1  =           T
PRWT   =           T
PRY    =           T
SIMULA =           T
LUSER  =           F           F           T           F           F           F           F           F           F           F
                   F           F           F           F           F           F           F           F           F           F
                   F           F           F           F           F           F           F           F           F           F

PRECIS = 1.86D-16          SRANGE = 1.00E+35      RANGE = 1.00D+35

SQUARED FORM FACTORS
   9.927E-01   9.908E-01   9.875E-01   9.830E-01   9.770E-01   9.688E-01   9.578E-01   9.431E-01   9.233E-01   8.970E-01
   8.623E-01   8.170E-01   7.587E-01   6.851E-01   5.950E-01   4.888E-01   3.706E-01   2.490E-01   1.383E-01   5.499E-02
   1.043E-02   9.464E-04   5.988E-03   5.516E-03   7.918E-04   8.086E-04   6.088E-04   1.999E-04   1.237E-04   9.535E-05
   2.602E-05
```

T	Y	EXACT	ERROR
8.00000E-05	6.96205E-01	6.96413E-01	-2.08080E-04
2.40000E-04	6.27346E-01	6.27103E-01	2.42949E-04
4.00000E-04	5.66856E-01	5.66772E-01	8.44002E-05
5.60000E-04	5.14232E-01	5.13934E-01	2.98560E-04
7.20000E-04	4.66978E-01	4.67399E-01	-4.20600E-04
8.80000E-04	4.26116E-01	4.26206E-01	-9.04799E-05
1.04000E-03	3.90167E-01	3.89577E-01	5.89669E-04
1.20000E-03	3.56839E-01	3.56874E-01	-3.44515E-05
1.36000E-03	3.27530E-01	3.27571E-01	-4.02927E-05
1.52000E-03	3.00938E-01	3.01233E-01	-2.94566E-04
1.68000E-03	2.77428E-01	2.77496E-01	-6.82175E-05
1.84000E-03	2.56419E-01	2.56053E-01	3.66479E-04
2.00000E-03	2.37001E-01	2.36643E-01	3.58164E-04
2.16000E-03	2.18723E-01	2.19042E-01	-3.19228E-04
2.32000E-03	2.02305E-01	2.03060E-01	-7.54476E-04
2.48000E-03	1.88383E-01	1.88527E-01	-1.43856E-04
2.64000E-03	1.75973E-01	1.75300E-01	6.73547E-04
2.80000E-03	1.63770E-01	1.63248E-01	5.21913E-04
2.96000E-03	1.51740E-01	1.52261E-01	-5.20825E-04
3.12000E-03	1.41746E-01	1.42237E-01	-4.90874E-04
3.28000E-03	1.32082E-01	1.33086E-01	-1.00362E-03
3.44000E-03	1.23611E-01	1.24729E-01	-1.11817E-03
3.60000E-03	1.17317E-01	1.17094E-01	2.22884E-04
3.76000E-03	1.07865E-01	1.10116E-01	-2.25133E-03
3.92000E-03	1.04093E-01	1.03738E-01	3.54953E-04
4.08000E-03	9.76379E-02	9.79049E-02	-2.66984E-04
4.24000E-03	9.26860E-02	9.25706E-02	1.15350E-04
4.40000E-03	8.70941E-02	8.76913E-02	-5.97179E-04
4.56000E-03	8.36017E-02	8.32275E-02	3.74243E-04
4.72000E-03	7.89098E-02	7.91434E-02	-2.33673E-04
4.88000E-03	7.74120E-02	7.54064E-02	2.00560E-03
5.04000E-03	6.85593E-02	7.19867E-02	-3.42742E-03
5.20000E-03	6.88957E-02	6.88571E-02	3.85791E-05
5.36000E-03	6.51086E-02	6.59928E-02	-8.84175E-04
5.52000E-03	6.35057E-02	6.33713E-02	1.34416E-04
5.68000E-03	6.19119E-02	6.09718E-02	9.40081E-04
5.84000E-03	5.90049E-02	5.87755E-02	2.29407E-04
6.00000E-03	5.82624E-02	5.67651E-02	1.49725E-03
6.16000E-03	5.72981E-02	5.49249E-02	2.37321E-03
6.32000E-03	5.41858E-02	5.32403E-02	9.45494E-04
6.48000E-03	4.80286E-02	5.16983E-02	-3.66973E-03
6.64000E-03	4.91268E-02	5.02867E-02	-1.15986E-03
6.80000E-03	4.99570E-02	4.89945E-02	9.62514E-04
6.96000E-03	4.61133E-02	4.78115E-02	-1.69816E-03

T	Y	EXACT	ERROR
1.60000E-04	6.60309E-01	6.60530E-01	-2.20180E-04
3.20000E-04	5.95803E-01	5.95916E-01	-1.12653E-04
4.80000E-04	5.39921E-01	5.39497E-01	4.24385E-04
6.40000E-04	4.89997E-01	4.89943E-01	5.38230E-05
8.00000E-04	4.45780E-01	4.46187E-01	-4.07189E-04
9.60000E-04	4.07596E-01	4.07364E-01	2.31534E-04
1.12000E-03	3.73083E-01	3.72770E-01	3.13073E-04
1.28000E-03	3.41805E-01	3.41826E-01	-2.10106E-05
1.44000E-03	3.14611E-01	3.14055E-01	5.55158E-04
1.60000E-03	2.88172E-01	2.89060E-01	-8.88199E-04
1.76000E-03	2.66439E-01	2.66505E-01	-6.61910E-05
1.92000E-03	2.47265E-01	2.46108E-01	1.15611E-03
2.08000E-03	2.27554E-01	2.27629E-01	-7.54148E-05
2.24000E-03	2.11137E-01	2.10860E-01	2.76908E-04
2.40000E-03	1.94874E-01	1.95622E-01	-7.47651E-04
2.56000E-03	1.82624E-01	1.81759E-01	8.65459E-04
2.72000E-03	1.69370E-01	1.69134E-01	2.35870E-04
2.88000E-03	1.58420E-01	1.57628E-01	7.92101E-04
3.04000E-03	1.46275E-01	1.47134E-01	-8.59037E-04
3.20000E-03	1.36996E-01	1.37557E-01	-5.61118E-04
3.36000E-03	1.28652E-01	1.28813E-01	-1.61305E-04
3.52000E-03	1.20834E-01	1.20826E-01	8.02428E-06
3.68000E-03	1.13535E-01	1.13527E-01	8.12113E-06
3.84000E-03	1.06873E-01	1.06856E-01	1.76057E-05
4.00000E-03	1.00682E-01	1.00756E-01	-7.35819E-05
4.16000E-03	9.48239E-02	9.51783E-02	-3.54335E-04
4.32000E-03	9.05933E-02	9.00766E-02	5.16653E-04
4.48000E-03	8.38884E-02	8.54098E-02	-1.52135E-03
4.64000E-03	8.20693E-02	8.11401E-02	9.29132E-04
4.80000E-03	7.82570E-02	7.72335E-02	1.02354E-03
4.96000E-03	7.31261E-02	7.36587E-02	-5.32560E-04
5.12000E-03	6.94362E-02	7.03872E-02	-9.50985E-04
5.28000E-03	6.70901E-02	6.73933E-02	-3.03172E-04
5.44000E-03	6.46413E-02	6.46530E-02	-1.17868E-05
5.60000E-03	6.22243E-02	6.21450E-02	7.93263E-05
5.76000E-03	5.95538E-02	5.98494E-02	-2.95572E-04
5.92000E-03	5.67243E-02	5.77481E-02	-1.02383E-03
6.08000E-03	5.02315E-02	5.58247E-02	-5.59318E-03
6.24000E-03	5.54786E-02	5.40640E-02	1.41460E-03
6.40000E-03	5.09338E-02	5.24523E-02	-1.51847E-03
6.56000E-03	5.35623E-02	5.09769E-02	2.58543E-03
6.72000E-03	5.06416E-02	4.96263E-02	1.01526E-03
6.88000E-03	4.80998E-02	4.83899E-02	-2.90107E-04
7.04000E-03	4.83847E-02	4.72581E-02	1.12662E-03

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
1.0000E-06	0.0000D+00	3.76D-03	2.6194D-26	8.00D-05	7.221D+19
1.1659E-06	0.0000D+00	4.64D-03	2.1233D-25	8.00D-05	7.221D+19
1.3594E-06	0.0000D+00	5.36D-03	2.1199D-25	8.00D-05	7.221D+19
1.5849E-06	0.0000D+00	6.48D-03	8.3589D-25	8.00D-05	7.221D+19
1.8478E-06	2.3404D-38	7.04D-03	8.1458D-25	8.00D-05	7.221D+19
2.1544E-06	7.6299D-36	7.04D-03	3.1415D-24	8.00D-05	7.221D+19
2.5119E-06	3.2734D-34	7.04D-03	2.9979D-24	8.00D-05	7.221D+19
2.9286E-06	3.2348D-32	7.04D-03	1.1326D-23	8.00D-05	7.221D+19
3.4145E-06	4.9674D-31	7.04D-03	1.0580D-23	8.00D-05	7.221D+19
3.9811E-06	2.0236D-29	7.04D-03	3.9049D-23	8.00D-05	7.221D+19
4.6416E-06	1.4433D-28	7.04D-03	3.5513D-23	8.00D-05	7.221D+19
5.4117E-06	3.0170D-27	7.04D-03	1.2690D-22	8.00D-05	7.221D+19
6.3095E-06	1.1984D-26	7.04D-03	1.1079D-22	8.00D-05	7.221D+19
7.3564E-06	1.4890D-25	7.04D-03	3.7532D-22	8.00D-05	7.221D+19
8.5769E-06	3.6888D-25	7.04D-03	3.0504D-22	8.00D-05	7.221D+19
9.9999E-06	2.9455D-24	7.04D-03	9.3641D-22	8.00D-05	7.221D+19
1.1659E-05	4.7278D-24	7.04D-03	6.6203D-22	8.00D-05	7.221D+19

MAR 84 Page 34

1.3593E-05	2.3914D-23	7.04D-03	1.6575D-21	8.00D-05	7.221D+19
1.5849E-05	2.2588D-23	7.04D-03	8.5650D-22	8.00D-05	7.221D+19
1.8478E-05	5.6007D-23	7.04D-03	1.2659D-21	8.00D-05	7.221D+19
2.1544E-05	1.5379D-23	7.04D-03	2.2305D-22	8.00D-05	7.221D+19
2.5119E-05	7.5765D-24	7.04D-03	7.5103D-23	8.00D-05	7.221D+19
2.9286E-05	6.1619D-23	7.04D-03	4.4070D-22	8.00D-05	7.221D+19
3.4145E-05	2.7847D-22	7.04D-03	1.5053D-21	8.00D-05	7.221D+19
3.9810E-05	4.7081D-23	7.04D-03	2.0017D-22	8.00D-05	7.221D+19
4.6415E-05	2.1885D-22	7.04D-03	7.5729D-22	8.00D-05	7.221D+19
5.4116E-05	1.8203D-22	7.04D-03	5.2788D-22	8.00D-05	7.221D+19
6.3095E-05	2.5742D-22	7.04D-03	6.4154D-22	8.00D-05	7.221D+19
7.3563E-05	1.6785D-22	7.04D-03	3.6735D-22	8.00D-05	7.221D+19
8.5769E-05	5.3530D-22	7.04D-03	1.0480D-21	8.00D-05	7.221D+19
9.9999E-05	7.4330D-23	7.04D-03	1.3225D-22	8.00D-05	7.221D+19
NLINF TERMS	1.0000D+00	8.00D-05	1.0000D+00	8.00D-05	1.136D-02

MAR 84 Page 35

SCALE FACTOR FOR ALPHA = 1.179E-19

1 UNREGULARIZED VARIABLES

SINGULAR VALUES

7.268E+05	2.172E+00	1.092E-01	9.193E-03	9.054E-04	1.272E-04	1.896E-05	2.835E-06	4.503E-07	7.628E-08
1.355E-08	2.547E-09	1.057E-09	7.019E-10	4.617E-10	3.984E-10	3.260E-10	2.302E-10	2.224E-10	1.905E-10
1.636E-10	1.473E-10	1.237E-10	7.457E-11	4.552E-11	3.112E-11	1.422E-11	5.715E-12	1.334E-12	1.084E-12
5.843E-13	1.707E-13								

CONTIN - VERSION 2DP (MAR 1984) (PCS-1 PACK) TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

REFERENCES - S.W. PROVENCHER (1982) COMPUT. PHYS. COMMUN., VOL. 27, PAGES 213-227, 229-242.
(1984) EMBL TECHNICAL REPORT DA07 (EUROPEAN MOLECULAR BIOLOGY LABORATORY, HEIDELBERG, F.R. OF GERMANY)

MAR 84 Page 1

INPUT DATA FOR CHANGES TO COMMON VARIABLES

```
NG          0    2.10000E+01

GMNMX       1    5.00000E+02

GMNMX       2    5.00000E+06

NINTT       0    3.00000E+00

IFORMY      0    0.00000E+00
(6F8.6)

IUSER      10    1.00000E+00

RUSER      15    1.43000E+00

RUSER      16    4.88000E+02

RUSER      17    6.00000E+01

RUSER      18    1.37000E-04

RUSER      22   -5.00000E-01

RUSER      10   -1.00000E+00

RSVMNX      0    0.00000E+00
0.100E+05 0.100E-09 0.000E+00 0.000E+00

NQPROG      1    3.00000E+00

NORDER      0    3.00000E+00

NENDZ       1    1.00000E+00

ALPST       2    7.96200E-06

LSIGN       0    0.00000E+00
  -1    0    0    0   -1    3   -7   13    0    0    0    0    0    0    0    0

NFLAT       0    0.00000E+00
   0    0    0    0    3    0    0    0

SRMIN       0    5.00000E-04

NNSGN       2    2.00000E+00

NSGN        2    4.00000E+00

NSGN        1    2.00000E+00

MQPITR      0    9.00000E+01

END         0    0.00000E+00
NSTEND     17    5.00000E-06    8.50000E-05
NSTEND     16    9.50000E-05    2.45000E-04
NSTEND      4    2.65000E-04    3.25000E-04
```

MAR 84 Page 2

```
                                   FINAL VALUES OF CONTROL VARIABLES
DFMIN  = 2.00000E+00
SRMIN  = 5.00000E-04
ALPST  = 0.00000E+00 7.96200E-06
GMNMX  = 5.00000E+02 5.00000E+06
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+04 1.00000E-10 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00-1.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.43000E+00 4.88000E+02 6.00000E+01 1.37000E-04 0.00000E+00 1.84118E+05
         4.64422E+06-5.00000E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 -0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
IGRID  =           2
IQUAD  =           3
IUNIT  =          -1
IWT    =           1
LINEPG =          60
MIOERR =           5
MPKMOM =           5
MQPITR =          90
NEQ    =           0
NERFIT =          10
NG     =          21
NINTT  =           3
NLINF  =           0
NORDER =           3
ICRIT  =           1           1
IFORMT = (5E15.6)
IFORMW = (5E15.6)
IFORMY = (6F8.6)
IPLFIT =           2           2
IPLRES =           2           2
IPRINT =           4           4
IUSER  =           0           0           0           0           0           0           0           0           0           1
                   0           0           0           0           0           0           0          50           0           0
                   0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0           0           0           0           0
                   0           0           0           0           0           0           0           0           0           0
IUSROU =           0           0
LSIGN  =          -1           0           0           0          -1           3          -7          13           0           0
                   0           0           0           0           0           0
MOMNMX =          -1           3
NENDZ  =           1           2
NFLAT  =           0           0           0           0           3           0           0           0
NNSGN  =           0           2
NQPROG =           3           6
NSGN   =           2           4           0           0
DOCHOS =           T
DOMOM  =           T
DOUSIN =           T
DOUSNQ =           F
LAST   =           T
NEWPG1 =           F
NONNEG =           T
ONLY1  =           T
PRWT   =           T
PRY    =           T
SIMULA =           F
LUSER  =           F           F           F           F           F           F           F           F           F           F
                   F           F           F           F           F           F           F           F           F           F
                   F           F           F           F           F           F           F           F           F           F
```

T	Y	T	Y	T	Y	T	Y	T	Y
5.000E-06	6.71565E-01	1.000E-05	6.40401E-01	1.500E-05	6.10346E-01	2.000E-05	5.83154E-01	2.500E-05	5.57062E-01
3.000E-05	5.32512E-01	3.500E-05	5.08776E-01	4.000E-05	4.85827E-01	4.500E-05	4.65630E-01	5.000E-05	4.46515E-01
5.500E-05	4.26056E-01	6.000E-05	4.06806E-01	6.500E-05	3.92105E-01	7.000E-05	3.73747E-01	7.500E-05	3.58781E-01
8.000E-05	3.43080E-01	8.500E-05	3.31479E-01	9.500E-05	3.06780E-01	1.050E-04	2.83829E-01	1.150E-04	2.62155E-01
1.250E-04	2.42237E-01	1.350E-04	2.31004E-01	1.450E-04	2.12779E-01	1.550E-04	1.98950E-01	1.650E-04	1.83082E-01
1.750E-04	1.77724E-01	1.850E-04	1.67245E-01	1.950E-04	1.54842E-01	2.050E-04	1.47347E-01	2.150E-04	1.46741E-01
2.250E-04	1.42520E-01	2.350E-04	1.28402E-01	2.450E-04	1.31195E-01	2.650E-04	1.26795E-01	2.850E-04	1.07968E-01
3.050E-04	1.15698E-01	3.250E-04	1.03947E-01						

PRECIS = 1.86D-16 SRANGE = 1.00E+35 RANGE = 1.00D+35

MAR 84 Page 3

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
5.0000E+02	1.8565D-25	3.25D-04	1.3585D+04	5.00D-06	1.181D-13
7.9245E+02	1.9957D-18	3.25D-04	1.6900D+05	5.00D-06	6.748D-14
1.2559E+03	1.5429D-13	3.25D-04	2.5149D+05	5.00D-06	5.904D-14
1.9905E+03	4.9389D-09	3.25D-04	1.4457D+06	5.00D-06	5.904D-14
3.1548E+03	6.5228D-06	3.25D-04	2.0209D+06	5.00D-06	5.904D-14
5.0000E+03	8.2373D-03	3.25D-04	1.1054D+07	5.00D-06	5.904D-14
7.9245E+03	8.3446D-01	3.25D-04	1.4853D+07	5.00D-06	5.904D-14
1.2559E+04	1.3707D+02	3.25D-04	7.8729D+07	5.00D-06	5.904D-14
1.9905E+04	2.7474D+03	3.25D-04	1.0318D+08	5.00D-06	5.904D-14
3.1548E+04	1.2461D+05	3.25D-04	5.3622D+08	5.00D-06	5.904D-14
5.0000E+04	8.9858D+05	3.25D-04	6.9182D+08	5.00D-06	5.904D-14
7.9245E+04	1.8093D+07	3.25D-04	3.5506D+09	5.00D-06	5.904D-14
1.2559E+05	6.8457D+07	3.25D-04	4.5356D+09	5.00D-06	5.904D-14
1.9905E+05	8.2580D+08	3.25D-04	2.3095D+10	5.00D-06	5.904D-14
3.1548E+05	2.0798D+09	3.25D-04	2.9318D+10	5.00D-06	5.904D-14
5.0000E+05	1.8159D+10	3.25D-04	1.4855D+11	5.00D-06	5.904D-14
7.9245E+05	3.5377D+10	3.25D-04	1.8783D+11	5.00D-06	5.904D-14
1.2559E+06	2.5189D+11	3.25D-04	9.4869D+11	5.00D-06	5.904D-14
1.9905E+06	4.1733D+11	3.25D-04	1.1966D+12	5.00D-06	5.904D-14
3.1548E+06	2.6125D+12	3.25D-04	6.0318D+12	5.00D-06	5.904D-14
5.0000E+06	1.9539D+12	3.25D-04	3.7980D+12	5.00D-06	6.748D-14

SCALE FACTOR FOR ALPHA = 4.446E+13

0 UNREGULARIZED VARIABLES

SINGULAR VALUES

7.932E+00	8.282E-02	2.925E-03	1.730E-04	1.363E-05	1.309E-06	1.346E-07	1.614E-08	2.030E-09	7.769E-10
2.668E-10	1.147E-10	3.365E-11	1.183E-11	3.282E-12	1.252E-12	3.149E-13	9.649E-14	2.308E-14	5.684E-15
5.135E-16									

MAX. ITERATIONS IN NNLS FOR ALPHA/S(1) = 1.86E-12

MAX. ITERATIONS IN NNLS FOR ALPHA/S(1) = 1.36E-11

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 7.93E-10	1.00E-10	6.09237E-04	6.09237E-04	4.233E-03	3.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA	
0.000E+00	1.0D-28	5.00E+02X	
0.000E+00	1.6D-28	7.92E+02X	
0.000E+00	2.8D-28	1.26E+03X	
0.000E+00	4.0D-28	1.99E+03X	
0.000E+00	8.8D-29	3.15E+03X	
0.000E+00	4.9D-28	5.00E+03X	
0.000E+00	7.3D-29	7.92E+03X	
0.000E+00	6.5D-28	1.26E+04X	
0.000E+00	6.1D-28	1.99E+04X	
0.000E+00	4.4D-27	3.15E+04X	
0.000E+00	5.0D-29	5.00E+04X	
0.000E+00	1.7D-28	7.92E+04X	
8.729E-11	8.1D-12	1.26E+05	
4.802E-12	1.7D-12	1.99E+05	..X..
0.000E+00	9.6D-28	3.15E+05X	
0.000E+00	3.1D-27	5.00E+05X	
0.000E+00	9.7D-28	7.92E+05X	
0.000E+00	9.0D-28	1.26E+06X	
0.000E+00	7.7D-28	1.99E+06X	
0.000E+00	1.7D-27	3.15E+06X	
4.444E-14	1.2D-15	5.00E+06X	

MAR 84 Page 4

.....X

PEAK 1 GOES FROM 5.000E+02 TO 3.155E+06

(STD. DEV.)/MEAN = 1.9E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.9748 X (10** -11)	4.9E+00			
0	3.9528 X (10** -6)	2.7E+00	1.3287E+05	7.6E+00	0
1	5.3956 X (10** -1)	7.2E-01	1.3650E+05	3.4E+00	1
2	7.6346 X (10** 4)	4.4E+00	1.4150E+05	5.1E+00	2
3	1.1297 X (10** 10)	9.1E+00	1.4797E+05	1.3E+01	3

PEAK 2 GOES FROM 5.000E+06 TO 5.000E+06

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	6.8220 X (10** -15)	2.6E+00			
0	3.4110 X (10** -8)	2.6E+00	5.0000E+06	5.2E+00	0
1	1.7055 X (10** -1)	2.6E+00	5.0000E+06	5.2E+00	1
2	8.5275 X (10** 5)	2.6E+00	5.0000E+06	5.2E+00	2
3	4.2638 X (10** 12)	2.6E+00	5.0000E+06	5.2E+00	3

MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 2.5E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.9755 X (10** -11)	4.9E+00			
0	3.9869 X (10** -6)	2.7E+00	1.3399E+05	7.6E+00	0
1	7.1011 X (10** -1)	8.3E-01	1.7811E+05	3.5E+00	1
2	9.2910 X (10** 5)	2.4E+00	1.3084E+06	3.2E+00	2
3	4.2751 X (10** 12)	2.6E+00	4.6013E+06	5.0E+00	3

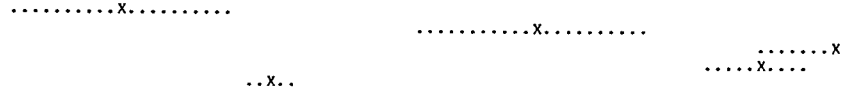
(FOR ALPHA/S(1) = 1.00E-10) PRUNS = 0.0105 PUNCOR = 0.0210 0.0450 0.0005 0.2231 0.9776

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
7.96E-06	1.00E-06	7.99880E-04	7.36866E-04	4.659E-03	3.059	0.913	1.000

MAR 84 Page 5

ORDINATE	ERROR	ABSCISSA
6.351E-13	1.9D-12	5.00E+02..X.....
1.045E-12	3.0D-12	7.92E+02...X.....
1.229E-12	3.3D-12	1.26E+03....X.....
1.186E-12	2.9D-12	1.99E+03....X.....
9.216E-13	2.0D-12	3.15E+03...X.....
4.720E-13	8.4D-13	5.00E+03.X...
0.000E+00	1.0D-28	7.92E+03X
0.000E+00	2.5D-29	1.26E+04X
2.040E-12	1.3D-12	1.99E+04 .....X.....
8.664E-12	2.7D-12	3.15E+04
1.899E-11	2.9D-12	5.00E+04
2.668E-11	2.1D-12	7.92E+04
2.464E-11	1.2D-12	1.26E+05
1.249E-11	4.9D-13	1.99E+05
1.048E-13	6.0D-13	3.15E+05X..
0.000E+00	5.3D-29	5.00E+05X
0.000E+00	7.0D-29	7.92E+05X
0.000E+00	7.0D-29	1.26E+06X
0.000E+00	2.8D-29	1.99E+06X
0.000E+00	4.2D-29	3.15E+06X
4.219E-14	1.3D-15	5.00E+06X



PEAK 1 GOES FROM 5.000E+02 TO 1.256E+04

(STD. DEV.)/MEAN = 5.3E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	2.4173 X (10** -12)	2.5E+02			
0	4.8220 X (10** -9)	2.3E+02	1.9948E+03	4.8E+02	0
1	1.3968 X (10** -5)	2.1E+02	2.8968E+03	4.3E+02	1
2	5.1930 X (10** -2)	1.9E+02	3.7177E+03	4.0E+02	2
3	2.2178 X (10** 2)	1.9E+02	4.2707E+03	3.8E+02	3

PEAK 2 GOES FROM 1.991E+04 TO 3.155E+06

(STD. DEV.)/MEAN = 4.5E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	4.3420 X (10** -11)	8.9E+00			
0	4.2563 X (10** -6)	3.7E+00	9.8027E+04	1.3E+01	0
1	5.4933 X (10** -1)	8.0E-01	1.2906E+05	4.5E+00	1
2	8.5528 X (10** 4)	4.7E+00	1.5569E+05	5.5E+00	2
3	1.4927 X (10** 10)	1.0E+01	1.7453E+05	1.5E+01	3

PEAK 3 GOES FROM 5.000E+06 TO 5.000E+06

(STD. DEV.)/MEAN = 1.7E-04

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	6.4770 X (10** -15)	3.0E+00			
0	3.2385 X (10** -8)	3.0E+00	5.0000E+06	6.0E+00	0
1	1.6192 X (10** -1)	3.0E+00	5.0000E+06	6.0E+00	1
2	8.0962 X (10** 5)	3.0E+00	5.0000E+06	6.0E+00	2
3	4.0481 X (10** 12)	3.0E+00	5.0000E+06	6.0E+00	3

MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 2.6E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	4.5843 X (10** -11)	1.6E+01			
0	4.2935 X (10** -6)	3.6E+00	9.3656E+04	1.9E+01	0
1	7.1127 X (10** -1)	9.2E-01	1.6566E+05	4.6E+00	1
2	8.9515 X (10** 5)	2.8E+00	1.2585E+06	3.7E+00	2
3	4.0631 X (10** 12)	3.0E+00	4.5389E+06	5.8E+00	3

(FOR ALPHA/S(1) = 1.00E-06) PRUNS = 0.0105 PUNCOR = 0.0031 0.0116 0.0002 0.1496 0.8836

1-EXTREMA-CONSTRAINED ANALYSIS

ALPHA = 7.96E-06 ALPHA/S(1) = 1.00E-06

MAR 84 Page 6

ITER.	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 REJ	PROB2 REJ	EXTREMA INDICES
* 1	9.666128E-04	9.15800E-04	5.186E-03	2.946	0.997	1.000	-1 12
2	1.021574E-03	9.29757E-04	5.211E-03	2.760	0.998	1.000	-1 13
3	9.813391E-04	9.38989E-04	5.245E-03	2.864	0.998	1.000	-1 11

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
7.96E-06	1.00E-06	9.66613E-04	9.15800E-04	5.186E-03	2.946	0.997	1.000

ORDINATE	ERROR	ABSCISSA
0.000E+00	5.3D-29	5.00E+02X
2.547E-25	1.5D-28	7.92E+02X
3.169E-25	8.3D-29	1.26E+03X
3.432E-25	2.2D-28	1.99E+03X
3.417E-25	3.6D-29	3.15E+03X
3.189E-25	3.6D-29	5.00E+03X
2.731E-25	3.2D-29	7.92E+03X
7.031E-13	1.4D-12	1.26E+04..X....
5.289E-12	3.4D-12	1.99E+04 ....X..........
1.472E-11	4.6D-12	3.15E+04
2.569E-11	4.3D-12	5.00E+04 ....X..............
3.080E-11	2.5D-12	7.92E+04
2.448E-11	5.0D-13	1.26E+05 ....X..............
1.033E-11	7.7D-13	1.99E+05 X
1.553E-14	3.8D-16	3.15E+05X ..X... ..X..
1.553E-14	3.8D-16	5.00E+05X
1.553E-14	3.8D-16	7.92E+05X
1.553E-14	3.8D-16	1.26E+06X
1.553E-14	3.8D-16	1.99E+06X
1.553E-14	3.8D-16	3.15E+06X
1.553E-14	3.8D-16	5.00E+06X

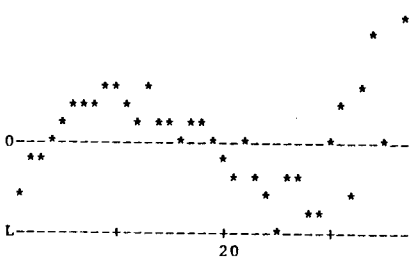
PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 2.3E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	5.1796 X (10** -11)	1.4E+01			
0	4.4954 X (10** -6)	4.9E+00	8.6790E+04	1.8E+01	0
1	7.1220 X (10** -1)	5.0E-01	1.5843E+05	5.4E+00	1
2	7.3306 X (10** 5)	1.8E+00	1.0293E+06	2.3E+00	2
3	2.5477 X (10** 12)	2.4E+00	3.4755E+06	4.2E+00	3

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

WEIGHTED RESIDUALS (ALPHA/S(1)= 1.00E-06) MAX=U= 1.6E-02 MIN=L=-8.9E-03 (PRUNS= 0.0016) PUNCOR= 0.0003 0.0024 0.0001 0.1027 0.7785



MAR 84 Page 7

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
6.767E-01	5.00E-06
6.435E-01	1.00E-05
6.124E-01	1.50E-05
5.832E-01	2.00E-05
5.559E-01	2.50E-05
5.302E-01	3.00E-05
5.060E-01	3.50E-05
4.834E-01	4.00E-05
4.620E-01	4.50E-05
4.420E-01	5.00E-05
4.231E-01	5.50E-05
4.053E-01	6.00E-05
3.886E-01	6.50E-05
3.728E-01	7.00E-05
3.579E-01	7.50E-05
3.438E-01	8.00E-05
3.305E-01	8.50E-05
3.061E-01	9.50E-05
2.842E-01	1.05E-04
2.646E-01	1.15E-04
2.470E-01	1.25E-04
2.311E-01	1.35E-04
2.168E-01	1.45E-04
2.038E-01	1.55E-04
1.920E-01	1.65E-04
1.813E-01	1.75E-04
1.715E-01	1.85E-04
1.626E-01	1.95E-04
1.544E-01	2.05E-04
1.469E-01	2.15E-04
1.400E-01	2.25E-04
1.336E-01	2.35E-04
1.277E-01	2.45E-04
1.171E-01	2.65E-04
1.080E-01	2.85E-04
1.000E-01	3.05E-04
9.294E-02	3.25E-04

1-EXTREMA-CONSTRAINED ANALYSIS

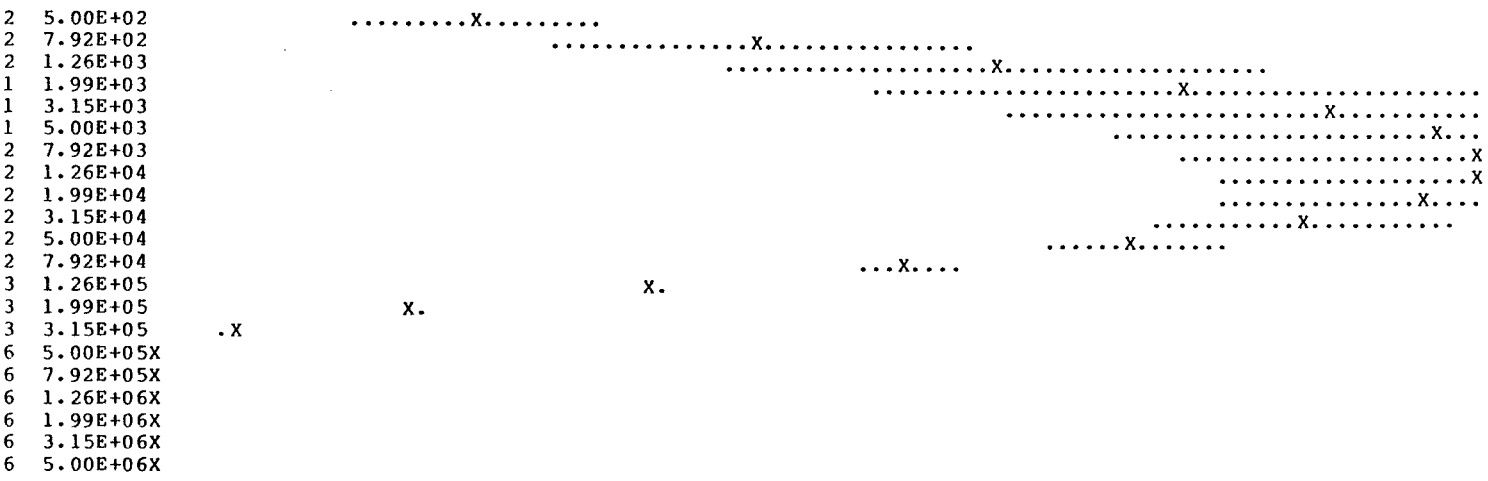
ALPHA = 5.83E-05 ALPHA/S(1) = 7.35E-06

ITER.	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 REJ	PROB2 REJ	EXTREMA INDICES
* 1	1.583253E-03	1.21454E-03	5.926E-03	2.414	1.000	1.000	-1 12
2	2.258250E-03	1.68925E-03	6.970E-03	2.229	1.000	1.000	-1 13
* 3	1.342398E-03	1.11757E-03	5.698E-03	2.583	1.000	1.000	-1 11
* 4	1.274397E-03	1.12404E-03	5.724E-03	2.694	1.000	1.000	-1 10
* 5	1.254723E-03	1.13950E-03	5.769E-03	2.762	1.000	1.000	-1 9
* 6	1.250149E-03	1.15139E-03	5.803E-03	2.808	1.000	1.000	-1 8
* 7	1.250136E-03	1.15202E-03	5.810E-03	2.872	1.000	1.000	-1 7
8	1.253414E-03	1.15990E-03	5.827E-03	2.844	1.000	1.000	-1 6

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
5.83E-05	7.35E-06	1.25014E-03	1.15202E-03	5.810E-03	2.872	1.000	1.000

ORDINATE	ERROR	ABSCISSA
1.086E-11	3.8D-12	5.00E+02
2.023E-11	6.8D-12	7.92E+02
2.811E-11	9.0D-12	1.26E+03
3.449E-11	1.0D-11	1.99E+03
3.934E-11	1.1D-11	3.15E+03
4.261E-11	1.1D-11	5.00E+03
4.424E-11	9.7D-12	7.92E+03
4.413E-11	8.4D-12	1.26E+04
4.218E-11	6.7D-12	1.99E+04
3.833E-11	4.8D-12	3.15E+04
3.258E-11	2.9D-12	5.00E+04
2.519E-11	1.4D-12	7.92E+04
1.681E-11	3.0D-13	1.26E+05
8.760E-12	3.1D-13	1.99E+05
2.710E-12	2.6D-13	3.15E+05
1.452E-14	4.2D-16	5.00E+05
1.452E-14	4.2D-16	7.92E+05
1.452E-14	4.2D-16	1.26E+06
1.452E-14	4.2D-16	1.99E+06
1.452E-14	4.2D-16	3.15E+06
1.452E-14	4.2D-16	5.00E+06



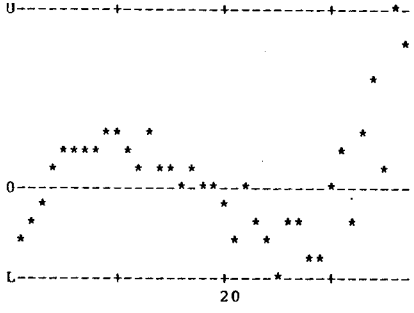
PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(STD. DEV.)/MEAN = 2.5E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9618 X (10** -10)	1.9E+01			
0	5.4553 X (10** -6)	6.3E+00	2.7808E+04	2.6E+01	0
1	7.1522 X (10** -1)	5.6E-01	1.3111E+05	6.9E+00	1
2	7.0319 X (10** 5)	2.1E+00	9.8318E+05	2.7E+00	2
3	2.3888 X (10** 12)	2.8E+00	3.3971E+06	5.0E+00	3

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

WEIGHTED RESIDUALS (ALPHA/S(1)= 7.35E-06) MAX=U= 1.7E-02 MIN=L=-9.7E-03 (PRUNS= 0.0002) PUNCOR= 0.0000 0.0004 0.0001 0.0653 0.6189



MAR 84 Page 9

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
6.784E-01	5.00E-06
6.442E-01	1.00E-05
6.124E-01	1.50E-05
5.827E-01	2.00E-05
5.551E-01	2.50E-05
5.293E-01	3.00E-05
5.051E-01	3.50E-05
4.825E-01	4.00E-05
4.612E-01	4.50E-05
4.413E-01	5.00E-05
4.226E-01	5.50E-05
4.049E-01	6.00E-05
3.884E-01	6.50E-05
3.727E-01	7.00E-05
3.580E-01	7.50E-05
3.441E-01	8.00E-05
3.309E-01	8.50E-05
3.067E-01	9.50E-05
2.850E-01	1.05E-04
2.655E-01	1.15E-04
2.480E-01	1.25E-04
2.321E-01	1.35E-04
2.177E-01	1.45E-04
2.047E-01	1.55E-04
1.928E-01	1.65E-04
1.819E-01	1.75E-04
1.720E-01	1.85E-04
1.629E-01	1.95E-04
1.546E-01	2.05E-04
1.469E-01	2.15E-04
1.398E-01	2.25E-04
1.333E-01	2.35E-04
1.272E-01	2.45E-04
1.163E-01	2.65E-04
1.069E-01	2.85E-04
9.858E-02	3.05E-04
9.129E-02	3.25E-04

3-EXTREMA-CONSTRAINED ANALYSIS

ALPHA = 7.96E-06 ALPHA/S(1) = 1.00E-06

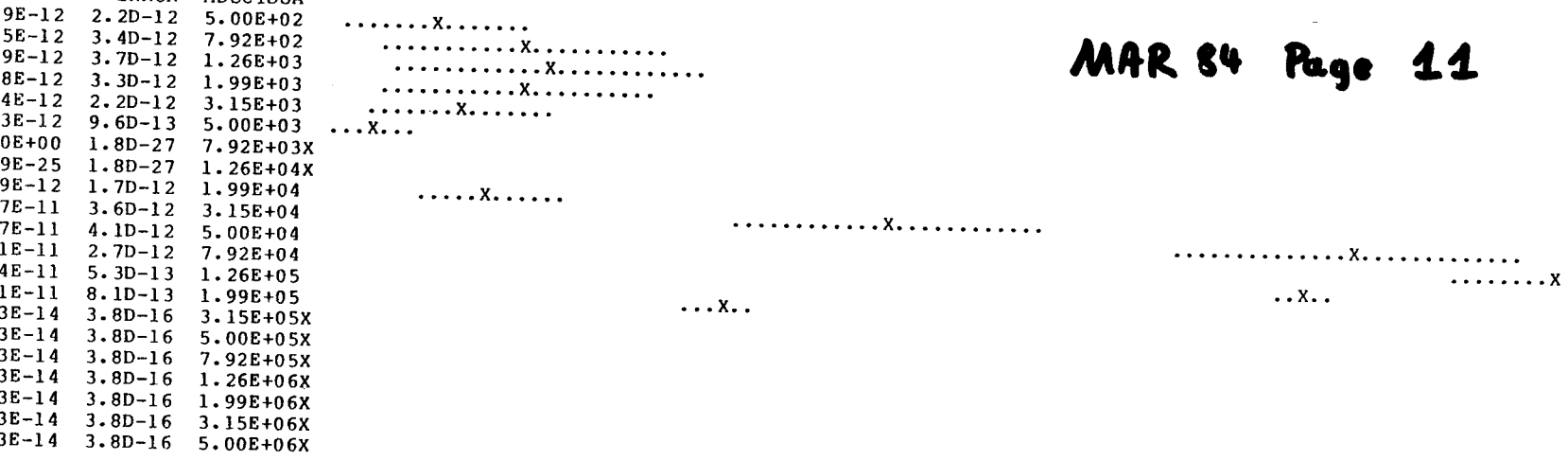
MAR 84 Page 10

	ITER.	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 REJ	PROB2 REJ	EXTREMA INDICES
*	1	1.021461E-03	9.29570E-04	5.206E-03	2.700	0.998	1.000	-1 3 -7 13
	2	1.518287E-03	1.34348E-03	6.196E-03	2.001	1.000	1.000	-1 3 -7 14
*	3	9.662192E-04	9.14514E-04	5.179E-03	2.908	0.997	1.000	-1 3 -7 12
	4	9.810354E-04	9.39574E-04	5.247E-03	2.866	0.998	1.000	-1 3 -7 11
	5	9.662192E-04	9.14514E-04	5.179E-03	2.908	0.997	1.000	-1 3 -8 12
	6	1.022733E-03	9.25992E-04	5.191E-03	2.630	0.998	1.000	-1 3 -8 13
	7	9.841478E-04	9.33938E-04	5.230E-03	2.855	0.998	1.000	-1 3 -8 11
	8	9.787359E-04	9.03618E-04	5.144E-03	2.844	0.996	1.000	-1 3 -9 12
	9	1.029307E-03	9.35156E-04	5.235E-03	2.876	0.998	1.000	-1 3 -9 13
	10	1.008737E-03	9.56365E-04	5.295E-03	2.895	0.999	1.000	-1 3 -9 11
X	11	9.662192E-04						-1 3 -7 12
X	12	1.021461E-03						-1 3 -7 13
X	13	9.810354E-04						-1 3 -7 11
	14	9.666043E-04	9.15945E-04	5.187E-03	2.951	0.997	1.000	-1 3 -6 12
	15	1.021461E-03	9.29570E-04	5.206E-03	2.700	0.998	1.000	-1 3 -6 13
	16	9.810354E-04	9.39574E-04	5.247E-03	2.866	0.998	1.000	-1 3 -6 11
	17	9.662626E-04	9.14376E-04	5.179E-03	2.907	0.997	1.000	-1 4 -7 12
	18	1.021495E-03	9.29454E-04	5.205E-03	2.697	0.998	1.000	-1 4 -7 13
	19	9.811068E-04	9.39411E-04	5.246E-03	2.865	0.998	1.000	-1 4 -7 11
	20	9.662626E-04	9.14376E-04	5.179E-03	2.907	0.997	1.000	-1 4 -8 12
	21	1.022791E-03	9.25885E-04	5.190E-03	2.629	0.998	1.000	-1 4 -8 13
	22	9.843146E-04	9.33734E-04	5.229E-03	2.854	0.998	1.000	-1 4 -8 11
	23	9.787404E-04	9.03583E-04	5.143E-03	2.844	0.996	1.000	-1 4 -9 12
	24	1.029177E-03	9.35563E-04	5.237E-03	2.886	0.998	1.000	-1 4 -9 13
	25	1.008268E-03	9.56740E-04	5.297E-03	2.896	0.999	1.000	-1 4 -9 11
X	26	9.662626E-04						-1 4 -7 12
X	27	1.021495E-03						-1 4 -7 13
X	28	9.811068E-04						-1 4 -7 11
	29	9.666049E-04	9.15922E-04	5.186E-03	2.950	0.997	1.000	-1 4 -6 12
	30	1.021495E-03	9.29454E-04	5.205E-03	2.697	0.998	1.000	-1 4 -6 13
	31	9.811068E-04	9.39411E-04	5.246E-03	2.865	0.998	1.000	-1 4 -6 11
	32	9.663213E-04	9.14325E-04	5.179E-03	2.907	0.997	1.000	-1 2 -7 12
	33	1.021462E-03	9.29570E-04	5.206E-03	2.700	0.998	1.000	-1 2 -7 13
	34	9.810362E-04	9.39574E-04	5.247E-03	2.866	0.998	1.000	-1 2 -7 11
	35	9.663213E-04	9.14325E-04	5.179E-03	2.907	0.997	1.000	-1 2 -8 12
	36	1.022840E-03	9.25873E-04	5.190E-03	2.629	0.998	1.000	-1 2 -8 13
	37	9.844569E-04	9.33722E-04	5.229E-03	2.854	0.998	1.000	-1 2 -8 11
	38	9.797688E-04	9.02307E-04	5.139E-03	2.839	0.996	1.000	-1 2 -9 12
	39	1.030221E-03	9.33886E-04	5.230E-03	2.853	0.998	1.000	-1 2 -9 13
	40	1.011001E-03	9.54576E-04	5.290E-03	2.892	0.999	1.000	-1 2 -9 11
X	41	9.663213E-04						-1 2 -7 12
X	42	1.021462E-03						-1 2 -7 13
X	43	9.810362E-04						-1 2 -7 11
	44	9.666046E-04	9.15944E-04	5.187E-03	2.951	0.997	1.000	-1 2 -6 12
	45	1.021462E-03	9.29570E-04	5.206E-03	2.700	0.998	1.000	-1 2 -6 13
	46	9.810362E-04	9.39574E-04	5.247E-03	2.866	0.998	1.000	-1 2 -6 11

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
7.96E-06	1.00E-06	9.66219E-04	9.14514E-04	5.179E-03	2.908	0.997	1.000

ORDINATE	ERROR	ABSCISSA
3.369E-12	2.2D-12	5.00E+02
5.345E-12	3.4D-12	7.92E+02
5.969E-12	3.7D-12	1.26E+03
5.368E-12	3.3D-12	1.99E+03
3.804E-12	2.2D-12	3.15E+03
1.743E-12	9.6D-13	5.00E+03
0.000E+00	1.8D-27	7.92E+03
1.629E-25	1.8D-27	1.26E+04
4.599E-12	1.7D-12	1.99E+04
1.437E-11	3.6D-12	3.15E+04
2.567E-11	4.1D-12	5.00E+04
3.091E-11	2.7D-12	7.92E+04
2.454E-11	5.3D-13	1.26E+05
1.031E-11	8.1D-13	1.99E+05
1.553E-14	3.8D-16	3.15E+05
1.553E-14	3.8D-16	5.00E+05
1.553E-14	3.8D-16	7.92E+05
1.553E-14	3.8D-16	1.26E+06
1.553E-14	3.8D-16	1.99E+06
1.553E-14	3.8D-16	3.15E+06
1.553E-14	3.8D-16	5.00E+06



MAR 84 Page 11

PEAK 1 GOES FROM 5.000E+02 TO 1.256E+04

(STD. DEV.)/MEAN = 5.6E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.1166 X (10** -11)	6.1E+01			
0	2.0757 X (10** -8)	6.0E+01	1.8590E+03	1.2E+02	0
1	5.6521 X (10** -5)	5.8E+01	2.7229E+03	1.2E+02	1
2	2.0178 X (10** -1)	5.7E+01	3.5700E+03	1.1E+02	2
3	8.4225 X (10** 2)	5.6E+01	4.1741E+03	1.1E+02	3

PEAK 2 GOES FROM 1.991E+04 TO 5.000E+06

(STD. DEV.)/MEAN = 2.3E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	5.1002 X (10** -11)	1.0E+01			
0	4.4840 X (10** -6)	4.3E+00	8.7918E+04	1.5E+01	0
1	7.1211 X (10** -1)	4.8E-01	1.5881E+05	4.8E+00	1
2	7.3310 X (10** 5)	1.8E+00	1.0295E+06	2.3E+00	2
3	2.5480 X (10** 12)	2.4E+00	3.4756E+06	4.2E+00	3

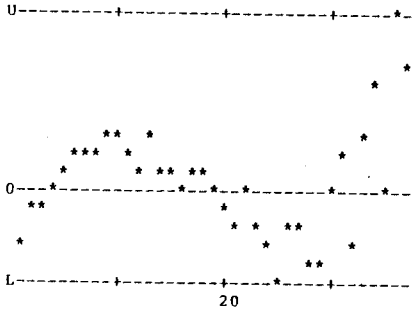
MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 2.3E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	6.2167 X (10** -11)	1.4E+01			
0	4.5047 X (10** -6)	4.3E+00	7.2461E+04	1.8E+01	0
1	7.1217 X (10** -1)	4.8E-01	1.5809E+05	4.8E+00	1
2	7.3311 X (10** 5)	1.8E+00	1.0294E+06	2.3E+00	2
3	2.5480 X (10** 12)	2.4E+00	3.4756E+06	4.2E+00	3

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

WEIGHTED RESIDUALS (ALPHA/S(1)= 1.00E-06) MAX=U= 1.6E-02 MIN=L=-8.9E-03 (PRUNS= 0.0016) PUNCOR= 0.0003 0.0024 0.0001 0.1028 0.7795



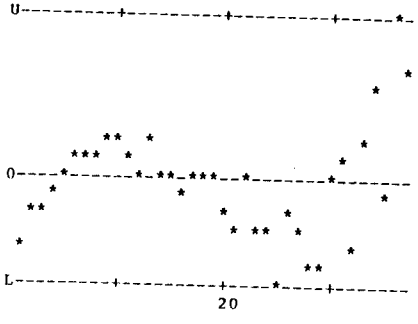
MAR 84 Page 12

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
6.767E-01	5.00E-06
6.435E-01	1.00E-05
6.124E-01	1.50E-05
5.832E-01	2.00E-05
5.559E-01	2.50E-05
5.302E-01	3.00E-05
5.061E-01	3.50E-05
4.834E-01	4.00E-05
4.621E-01	4.50E-05
4.420E-01	5.00E-05
4.231E-01	5.50E-05
4.053E-01	6.00E-05
3.886E-01	6.50E-05
3.728E-01	7.00E-05
3.579E-01	7.50E-05
3.438E-01	8.00E-05
3.305E-01	8.50E-05
3.061E-01	9.50E-05
2.842E-01	1.05E-04
2.646E-01	1.15E-04
2.470E-01	1.25E-04
2.311E-01	1.35E-04
2.168E-01	1.45E-04
2.038E-01	1.55E-04
1.920E-01	1.65E-04
1.813E-01	1.75E-04
1.715E-01	1.85E-04
1.626E-01	1.95E-04
1.544E-01	2.05E-04
1.469E-01	2.15E-04
1.400E-01	2.25E-04
1.336E-01	2.35E-04
1.277E-01	2.45E-04
1.171E-01	2.65E-04
1.080E-01	2.85E-04
1.000E-01	3.05E-04
9.294E-02	3.25E-04

CONTIN 2DP (MAR 84) (PCS-1) TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

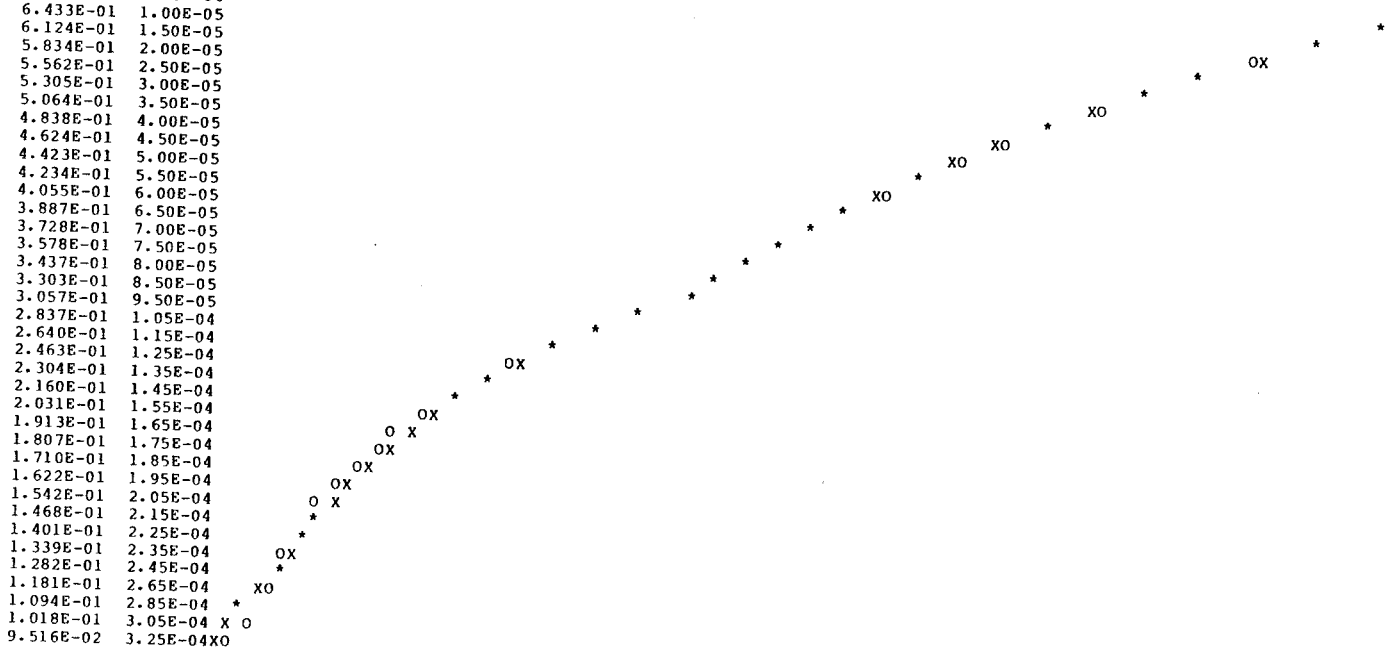
WEIGHTED RESIDUALS (ALPHA/S(1)= 1.00E-06) MAX=U= 1.4E-02 MIN=L=-8.3E-03 (PRUNS= 0.0105) PUNCOR= 0.0031 0.0116 0.0002 0.1496 0.8836 CHOSEN SOLUTION



MAR 84 Page 13

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
6.762E-01	5.00E-06
6.433E-01	1.00E-05
6.124E-01	1.50E-05
5.834E-01	2.00E-05
5.562E-01	2.50E-05
5.305E-01	3.00E-05
5.064E-01	3.50E-05
4.838E-01	4.00E-05
4.624E-01	4.50E-05
4.423E-01	5.00E-05
4.234E-01	5.50E-05
4.055E-01	6.00E-05
3.887E-01	6.50E-05
3.728E-01	7.00E-05
3.578E-01	7.50E-05
3.437E-01	8.00E-05
3.303E-01	8.50E-05
3.057E-01	9.50E-05
2.837E-01	1.05E-04
2.640E-01	1.15E-04
2.463E-01	1.25E-04
2.304E-01	1.35E-04
2.160E-01	1.45E-04
2.031E-01	1.55E-04
1.913E-01	1.65E-04
1.807E-01	1.75E-04
1.710E-01	1.85E-04
1.622E-01	1.95E-04
1.542E-01	2.05E-04
1.468E-01	2.15E-04
1.401E-01	2.25E-04
1.339E-01	2.35E-04
1.282E-01	2.45E-04
1.181E-01	2.65E-04
1.094E-01	2.85E-04
1.018E-01	3.05E-04
9.516E-02	3.25E-04



CONTIN VERSION 2DP (MAR 1984) (PCS-1 PACKAGE) ++++++++++++++++++++++++++++++++ CHOSEN SOLUTION ++++++++++++++++++++++++++++++++

TEST DATA SET 3 (FOR PEAK-CONSTRAINED SOLUTIONS)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
7.96E-06	1.00E-06	7.99880E-04	7.36866E-04	4.659E-03	3.059	0.913	1.000

MAR 84 Page 14

ORDINATE	ERROR	ABSCISSA
6.351E-13	1.9D-12	5.00E+02..X.....
1.045E-12	3.0D-12	7.92E+02...X.....
1.229E-12	3.3D-12	1.26E+03....X.....
1.186E-12	2.9D-12	1.99E+03....X.....
9.216E-13	2.0D-12	3.15E+03...X.....
4.720E-13	8.4D-13	5.00E+03.X...
0.000E+00	1.4D-29	7.92E+03X
0.000E+00	5.7D-29	1.26E+04X
2.040E-12	1.3D-12	1.99E+04 .....X.....
8.664E-12	2.7D-12	3.15E+04
1.899E-11	2.9D-12	5.00E+04
2.668E-11	2.1D-12	7.92E+04
2.464E-11	1.2D-12	1.26E+05
1.249E-11	4.9D-13	1.99E+05
1.048E-13	6.0D-13	3.15E+05X..
0.000E+00	2.5D-29	5.00E+05X
0.000E+00	5.0D-29	7.92E+05X
0.000E+00	4.7D-29	1.26E+06X
0.000E+00	2.4D-29	1.99E+06X
0.000E+00	3.3D-29	3.15E+06X
4.219E-14	1.3D-15	5.00E+06X

.....X.....

.....X.....

..X..

.....X.....

.....X

.....X....

	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
PEAK 1 GOES FROM 5.000E+02 TO 1.256E+04	-1	2.4173 X (10** -12)	2.5E+02			
	0	4.8220 X (10** -9)	2.3E+02	1.9948E+03	4.8E+02	0
	1	1.3968 X (10** -5)	2.1E+02	2.8968E+03	4.3E+02	1
(STD. DEV.)/MEAN = 5.3E-01	2	5.1930 X (10** -2)	1.9E+02	3.7177E+03	4.0E+02	2
	3	2.2178 X (10** 2)	1.9E+02	4.2707E+03	3.8E+02	3

	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
PEAK 2 GOES FROM 1.991E+04 TO 3.155E+06	-1	4.3420 X (10** -11)	8.9E+00			
	0	4.2563 X (10** -6)	3.7E+00	9.8027E+04	1.3E+01	0
	1	5.4933 X (10** -1)	8.0E-01	1.2906E+05	4.5E+00	1
(STD. DEV.)/MEAN = 4.5E-01	2	8.5528 X (10** 4)	4.7E+00	1.5569E+05	5.5E+00	2
	3	1.4927 X (10** 10)	1.0E+01	1.7453E+05	1.5E+01	3

	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
PEAK 3 GOES FROM 5.000E+06 TO 5.000E+06	-1	6.4770 X (10** -15)	3.0E+00			
	0	3.2385 X (10** -8)	3.0E+00	5.0000E+06	6.0E+00	0
	1	1.6192 X (10** -1)	3.0E+00	5.0000E+06	6.0E+00	1
(STD. DEV.)/MEAN = 1.7E-04	2	8.0962 X (10** 5)	3.0E+00	5.0000E+06	6.0E+00	2
	3	4.0481 X (10** 12)	3.0E+00	5.0000E+06	6.0E+00	3

	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
MOMENTS OF ENTIRE SOLUTION	-1	4.5843 X (10** -11)	1.6E+01			
	0	4.2935 X (10** -6)	3.6E+00	9.3656E+04	1.9E+01	0
	1	7.1127 X (10** -1)	9.2E-01	1.6566E+05	4.6E+00	1
(STD. DEV.)/MEAN = 2.6E+00	2	8.9515 X (10** 5)	2.8E+00	1.2585E+06	3.7E+00	2
	3	4.0631 X (10** 12)	3.0E+00	4.5389E+06	5.8E+00	3

CONTIN - VERSION 2DP (MAR 1984) (FBS-1 PACK) TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

REFERENCES - S.W. PROVENCHER (1982) COMPUT. PHYS. COMMUN., VOL. 27, PAGES 213-227, 229-242.
(1984) EMBL TECHNICAL REPORT DA07 (EUROPEAN MOLECULAR BIOLOGY LABORATORY, HEIDELBERG, F.R. OF GERMANY)

INPUT DATA FOR CHANGES TO COMMON VARIABLES

GMNMX	2	4.05000E+01	
NG	0	2.80000E+01	
NEQ	0	1.00000E+00	
NENDZ	1	0.00000E+00	
DOUSNQ	0	1.00000E+00	
RUSER	12	-1.00000E-02	
IWT	0	5.00000E+00	
RUSER	11	2.00000E+00	
NERFIT	0	0.00000E+00	
IFORMY (5F14.6)	0	0.00000E+00	
END	0	0.00000E+00	
NSTEND	61	1.60000E-02	7.60000E-02

MAR 84 Page 1

MAR 84 Page 2

```
                                          FINAL VALUES OF CONTROL VARIABLES
DFMIN  = 2.00000E+00
SRMIN  = 1.00000E-02
ALPST  = 0.00000E+00 0.00000E+00
GMNMX  = 0.00000E+00 4.05000E+01
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         2.00000E+00-1.00000E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
IGRID  =              1
IQUAD  =              3
IUNIT  =             -1
IWT    =              5
LINEPG =             60
MIOERR =              5
MPKMOM =              4
MQPITR =             35
NEQ    =              1
NERFIT =              0
NG     =             28
NINTT  =              1
NLINF  =              0
NORDER =              2
ICRIT  =              1            1
IFORMT = (5E15.6)
IFORMW = (5E15.6)
IFORMY = (5F14.6)
IPLFIT =              2            2
IPLRES =              2            2
IPRINT =              4            4
IUSER  =              0            0            0            0            0            0            0            0            0            2
                      0            0            0            0            0            0            0           50            0            0
                      0            0            0            0            0            0            0            0            0            0
                      0            0            0            0            0            0            0            0            0            0
                      0            0            0            0            0            0            0            0            0            0
IUSROU =              0            0
LSIGN  =              0            0            0            0            0            0            0            0            0            0
                      0            0            0            0            0            0
MOMNMX =              0            3
NENDZ  =              0            2
NFLAT  =              0            0            0            0            0            0            0            0
NNSGN  =              0            0
NQPROG =              6            6
NSGN   =              0            0            0            0
DOCHOS =              T
DOMOM  =              T
DOUSIN =              F
DOUSNQ =              T
LAST   =              T
NEWPG1 =              F
NONNEG =              F
ONLY1  =              T
PRWT   =              T
PRY    =              T
SIMULA =              F
LUSER  =              F            F            F            F            F            F            F            F            F            F
                      F            F            F            F            F            F            F            F            F            F
                      F            F            F            F            F            F            F            F            F            F
```

T	Y	T	Y	T	Y	T	Y	T	Y
1.600E-02	1.52331E+00	1.700E-02	1.19011E+00	1.800E-02	8.14006E-01	1.900E-02	5.35417E-01	2.000E-02	-4.02695E-01
2.100E-02	-5.67089E-01	2.200E-02	-7.51270E-01	2.300E-02	-9.48299E-01	2.400E-02	-1.11816E+00	2.500E-02	-1.25478E+00
2.600E-02	-1.37847E+00	2.700E-02	-1.46004E+00	2.800E-02	-1.47899E+00	2.900E-02	-1.46502E+00	3.000E-02	-1.43447E+00
3.100E-02	-1.35110E+00	3.200E-02	-1.27832E+00	3.300E-02	-1.16045E+00	3.400E-02	-1.03728E+00	3.500E-02	-8.95879E-01
3.600E-02	-7.22611E-01	3.700E-02	-6.03666E-01	3.800E-02	-4.35656E-01	3.900E-02	-2.83385E-01	4.000E-02	-1.93872E-01
4.100E-02	7.71920E-02	4.200E-02	2.70718E-01	4.300E-02	3.81172E-01	4.400E-02	4.50668E-01	4.500E-02	4.37786E-01
4.600E-02	5.15502E-01	4.700E-02	5.25926E-01	4.800E-02	5.36378E-01	4.900E-02	4.59074E-01	5.000E-02	4.10563E-01
5.100E-02	4.02334E-01	5.200E-02	3.47775E-01	5.300E-02	2.42373E-01	5.400E-02	0.00000E+00	5.500E-02	1.89404E-01
5.600E-02	0.00000E+00	5.700E-02	0.00000E+00	5.800E-02	0.00000E+00	5.900E-02	0.00000E+00	6.000E-02	-2.43996E-01
6.100E-02	-3.93584E-01	6.200E-02	-4.12606E-01	6.300E-02	-4.66926E-01	6.400E-02	-4.75384E-01	6.500E-02	-4.68763E-01
6.600E-02	-5.06462E-01	6.700E-02	-5.42777E-01	6.800E-02	-5.78173E-01	6.900E-02	-5.48281E-01	7.000E-02	-5.18167E-01
7.100E-02	-5.75197E-01	7.200E-02	-4.85255E-01	7.300E-02	-4.02439E-01	7.400E-02	-4.71114E-01	7.500E-02	-4.11118E-01
7.600E-02	-2.00000E-01								

PRECIS = 1.86D-16 SRANGE = 1.00E+35 RANGE = 1.00D+35

MAR 84 Page 3

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
0.0000E+00	0.0000D+00	1.60D-02	0.0000D+00	1.60D-02	1.664D-03
1.5000E+00	1.6508D+01	7.60D-02	1.8743D+01	1.60D-02	5.547D-04
3.0000E+00	1.0351D+01	7.60D-02	1.8423D+01	1.60D-02	4.161D-04
4.5000E+00	7.8590D+00	7.60D-02	5.3692D+01	1.60D-02	4.161D-04
6.0000E+00	-7.9548D+00	7.60D-02	3.4347D+01	1.60D-02	4.161D-04
7.5000E+00	-3.6749D+01	7.60D-02	8.1322D+01	1.60D-02	4.161D-04
9.0000E+00	-2.2773D+01	6.80D-02	4.5554D+01	1.60D-02	4.161D-04
1.0500E+01	-5.3142D+01	5.80D-02	9.7674D+01	1.60D-02	4.161D-04
1.2000E+01	-3.0365D+01	5.10D-02	5.0362D+01	1.60D-02	4.161D-04
1.3500E+01	-6.8319D+01	4.50D-02	1.0007D+02	1.60D-02	4.161D-04
1.5000E+01	-3.7939D+01	4.10D-02	4.7819D+01	1.60D-02	4.161D-04
1.6500E+01	-8.3509D+01	3.70D-02	8.7449D+01	1.60D-02	4.161D-04
1.8000E+01	-4.5547D+01	3.40D-02	3.7823D+01	1.60D-02	4.161D-04
1.9500E+01	-9.8638D+01	3.10D-02	7.3504D+01	5.70D-02	4.161D-04
2.1000E+01	-5.3142D+01	2.90D-02	3.9589D+01	5.30D-02	4.161D-04
2.2500E+01	-1.1387D+02	2.70D-02	8.4737D+01	5.00D-02	4.161D-04
2.4000E+01	-6.0618D+01	2.50D-02	4.5140D+01	4.70D-02	4.161D-04
2.5500E+01	-1.2905D+02	2.40D-02	9.6114D+01	4.40D-02	4.161D-04
2.7000E+01	-6.8159D+01	2.30D-02	5.0821D+01	4.10D-02	4.161D-04
2.8500E+01	-1.4388D+02	2.10D-02	1.0743D+02	3.90D-02	4.161D-04
3.0000E+01	-7.5773D+01	2.00D-02	5.6522D+01	3.70D-02	4.161D-04
3.1500E+01	-1.5902D+02	1.90D-02	1.1833D+02	3.50D-02	4.161D-04
3.3000E+01	-8.3094D+01	1.80D-02	6.2191D+01	3.40D-02	4.161D-04
3.4500E+01	-1.7419D+02	1.80D-02	1.2971D+02	3.20D-02	4.161D-04
3.6000E+01	-9.1094D+01	1.70D-02	6.7884D+01	3.10D-02	4.161D-04
3.7500E+01	-1.8943D+02	1.60D-02	1.4123D+02	3.00D-02	4.161D-04
3.9000E+01	-1.2288D+02	1.60D-02	9.1551D+01	2.90D-02	4.161D-04
4.0500E+01	-7.4712D+01	1.60D-02	5.6936D+01	2.80D-02	4.161D-04

SCALE FACTOR FOR ALPHA = 1.682E+04

0 UNREGULARIZED VARIABLES

SINGULAR VALUES

3.824E+00	1.098E+00	4.969E-01	2.369E-01	1.355E-01	8.111E-02	2.376E-02	2.625E-03	1.975E-04	1.265E-05
5.441E-07	1.734E-08	3.805E-09	2.647E-09	2.119E-09	1.983E-09	1.722E-09	1.345E-09	1.027E-09	8.880E-10
7.694E-10	5.683E-10	4.694E-10	3.595E-10	2.334E-10	1.119E-10	3.297E-17			

TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 7.12E-16	1.86E-16	3.95176E-01	3.95133E-01	8.717E-02	9.002	0.000	1.000

ORDINATE	ERROR	ABSCISSA
5.451E+08	3.4D+08	0.00E+00
-1.000E-02	1.5D-18	1.50E+00X
-1.000E-02	2.0D-18	3.00E+00X
-1.000E-02	2.2D-18	4.50E+00X
4.975E-02	5.7D-02	6.00E+00X
1.039E-02	3.3D-02	7.50E+00X
-1.000E-02	1.1D-17	9.00E+00X
-1.000E-02	3.8D-18	1.05E+01X
-1.000E-02	8.5D-18	1.20E+01X
-1.000E-02	8.7D-18	1.35E+01X
8.536E-02	9.2D-02	1.50E+01X
7.651E-04	4.5D-02	1.65E+01X
-1.000E-02	3.7D-18	1.80E+01X
-1.000E-02	1.4D-17	1.95E+01X
-1.000E-02	2.5D-17	2.10E+01X
-1.000E-02	7.2D-18	2.25E+01X
8.749E-02	6.9D-02	2.40E+01X
1.630E-03	3.1D-02	2.55E+01X
-1.000E-02	4.9D-17	2.70E+01X
-1.000E-02	1.7D-17	2.85E+01X
-1.000E-02	3.3D-17	3.00E+01X
-1.000E-02	2.9D-17	3.15E+01X
6.579E-02	3.0D-02	3.30E+01X
-6.636E-03	1.3D-02	3.45E+01X
-1.000E-02	1.6D-17	3.60E+01X
-1.000E-02	1.7D-17	3.75E+01X
1.285E-02	2.8D-03	3.90E+01X
0.000E+00	0.0D+00	4.05E+01X

.....X

MAR 84 Page 4

PEAK 1 GOES FROM 0.000E+00 TO 4.050E+01

(STD. DEV.)/MEAN = 6.5E+04

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	2.7257 X (10** 8)	6.2E+01			
1	1.3327 X (10** 0)	9.9E+00	4.8894E-09	7.2E+01	1
2	2.7895 X (10** 1)	1.2E+01	2.0931E+01	2.2E+01	2
3	6.4792 X (10** 2)	1.6E+01	2.3227E+01	2.8E+01	3

(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.0027

PUNCOR = 0.2785 0.2001 0.0535 0.6076 0.1464

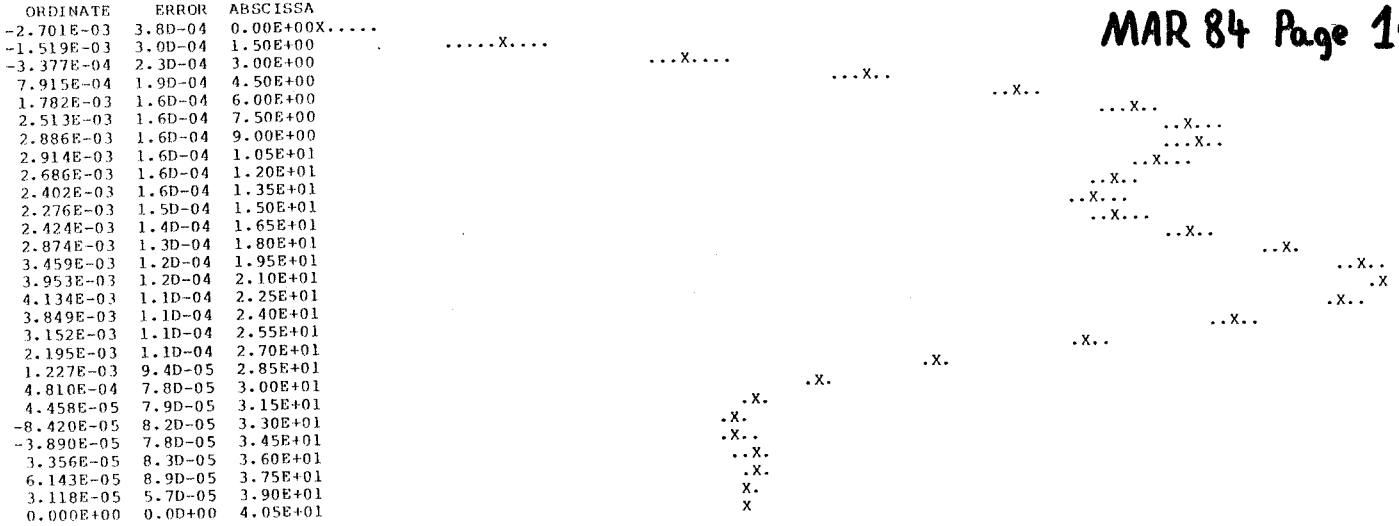
TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
2.20E-02	5.75E-03	6.44263E-01	4.45629E-01	9.038E-02	6.448	0.328	0.929

MAR 84 Page 14

ORDINATE	ERROR	ABSCISSA
-2.701E-03	3.8D-04	0.00E+00
-1.519E-03	3.0D-04	1.50E+00
-3.377E-04	2.3D-04	3.00E+00
7.915E-04	1.9D-04	4.50E+00
1.782E-03	1.6D-04	6.00E+00
2.513E-03	1.6D-04	7.50E+00
2.886E-03	1.6D-04	9.00E+00
2.914E-03	1.6D-04	1.05E+01
2.686E-03	1.6D-04	1.20E+01
2.402E-03	1.6D-04	1.35E+01
2.276E-03	1.5D-04	1.50E+01
2.424E-03	1.4D-04	1.65E+01
2.874E-03	1.3D-04	1.80E+01
3.459E-03	1.2D-04	1.95E+01
3.953E-03	1.2D-04	2.10E+01
4.134E-03	1.1D-04	2.25E+01
3.849E-03	1.1D-04	2.40E+01
3.152E-03	1.1D-04	2.55E+01
2.195E-03	1.1D-04	2.70E+01
1.227E-03	9.4D-05	2.85E+01
4.810E-04	7.8D-05	3.00E+01
4.458E-05	7.9D-05	3.15E+01
-8.420E-05	8.2D-05	3.30E+01
-3.890E-05	7.8D-05	3.45E+01
3.356E-05	8.3D-05	3.60E+01
6.143E-05	8.9D-05	3.75E+01
3.118E-05	5.7D-05	3.90E+01
0.000E+00	0.0D+00	4.05E+01



PEAK 1 GOES FROM 0.000E+00 TO 1.500E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	2.2146 X (10** -2)	1.1E+01			
1	2.6834 X (10** -1)	6.7E+00	1.2117E+01	1.8E+01	1
2	3.0199 X (10** 0)	6.1E+00	1.1254E+01	1.3E+01	2
3	3.5625 X (10** 1)	6.0E+00	1.1797E+01	1.2E+01	3

PEAK 2 GOES FROM 1.650E+01 TO 3.300E+01

(STD. DEV.)/MEAN = 1.6E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	4.2148 X (10** -2)	3.9E+00			
1	9.3244 X (10** -1)	4.1E+00	2.2123E+01	8.1E+00	1
2	2.1150 X (10** 1)	4.5E+00	2.2682E+01	8.6E+00	2
3	4.9111 X (10** 2)	4.9E+00	2.3221E+01	9.4E+00	3

PEAK 3 GOES FROM 3.450E+01 TO 4.050E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	1.1758 X (10** -4)	3.6E+02			
1	4.6509 X (10** -3)	3.4E+02	3.9554E+01	7.0E+02	1
2	1.8293 X (10** -1)	3.1E+02	3.9332E+01	6.5E+02	2
3	7.1614 X (10** 0)	2.9E+02	3.9148E+01	6.1E+02	3

MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 2.8E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	6.4411 X (10** -2)	4.7E+00			
1	1.2054 X (10** 0)	3.8E+00	1.8715E+01	8.5E+00	1
2	2.4352 X (10** 1)	4.6E+00	2.0202E+01	8.4E+00	2
3	5.3390 X (10** 2)	6.0E+00	2.1924E+01	1.1E+01	3

(FOR ALPHA/S(1) = 5.75E-03) PRUNS = 0.0000 PUNCOR = 0.0818 0.6547 0.2590 0.7581 0.2042

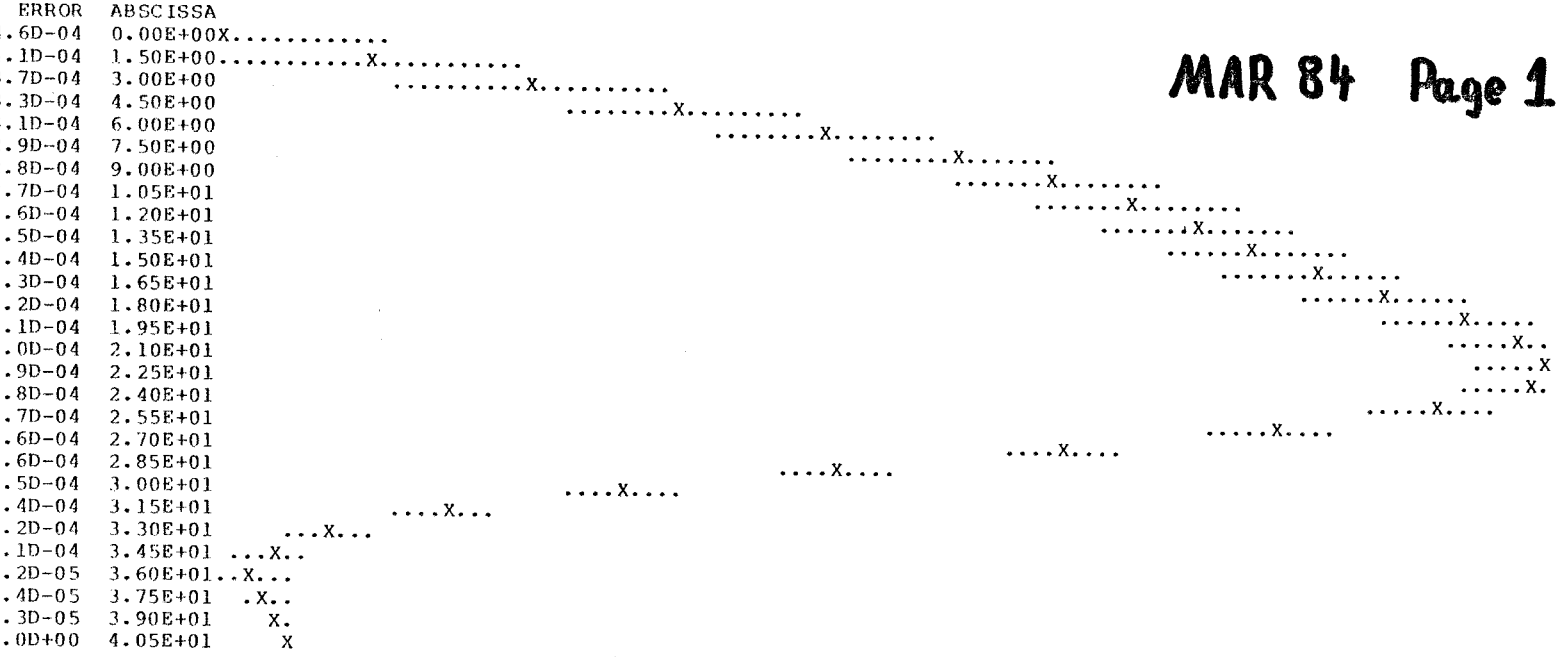
TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.63E-01	4.26E-02	4.11118E+00	2.33643E+00	2.028E-01	4.186	1.000	1.000

MAR 84 Page 15

ORDINATE	ERROR	ABSCISSA
2.197E-04	4.6D-04	0.00E+00
2.236E-04	4.1D-04	1.50E+00
6.670E-04	3.7D-04	3.00E+00
1.101E-03	3.3D-04	4.50E+00
1.510E-03	3.1D-04	6.00E+00
1.871E-03	2.9D-04	7.50E+00
2.166E-03	2.8D-04	9.00E+00
2.396E-03	2.7D-04	1.05E+01
2.574E-03	2.6D-04	1.20E+01
2.732E-03	2.5D-04	1.35E+01
2.904E-03	2.4D-04	1.50E+01
3.099E-03	2.3D-04	1.65E+01
3.311E-03	2.2D-04	1.80E+01
3.489E-03	2.1D-04	1.95E+01
3.573E-03	2.0D-04	2.10E+01
3.501E-03	1.9D-04	2.25E+01
3.232E-03	1.8D-04	2.40E+01
2.778E-03	1.7D-04	2.55E+01
2.182E-03	1.6D-04	2.70E+01
1.533E-03	1.6D-04	2.85E+01
9.259E-04	1.5D-04	3.00E+01
4.328E-04	1.4D-04	3.15E+01
1.038E-04	1.2D-04	3.30E+01
-6.778E-05	1.1D-04	3.45E+01
-1.119E-04	8.2D-05	3.60E+01
-8.269E-05	5.4D-05	3.75E+01
-3.389E-05	2.3D-05	3.90E+01
0.000E+00	0.0D+00	4.05E+01



PEAK 1 GOES FROM 0.000E+00 TO 3.600E+01

(STD. DEV.)/MEAN = 3.9E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	6.9107 X (10** -2)	1.1E+01			
1	1.2136 X (10** 0)	9.0E+00	1.7561E+01	2.0E+01	1
2	2.4630 X (10** 1)	9.6E+00	2.0295E+01	1.9E+01	2
3	5.4444 X (10** 2)	1.1E+01	2.2105E+01	2.0E+01	3

PEAK 2 GOES FROM 3.750E+01 TO 4.050E+01

(STD. DEV.)/MEAN = 1.6E-02

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	-2.0775 X (10** -4)	6.5E+01			
1	-7.8541 X (10** -3)	6.6E+01	3.7806E+01	1.3E+02	1
2	-2.9701 X (10** -1)	6.6E+01	3.7816E+01	1.3E+02	2
3	-1.1234 X (10** 1)	6.6E+01	3.7825E+01	1.3E+02	3

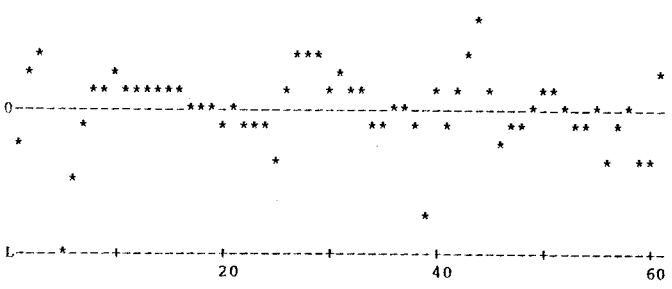
MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 3.9E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	6.8899 X (10** -2)	1.1E+01			
1	1.2058 X (10** 0)	9.1E+00	1.7500E+01	2.0E+01	1
2	2.4333 X (10** 1)	9.7E+00	2.0181E+01	1.9E+01	2
3	5.3321 X (10** 2)	1.1E+01	2.1913E+01	2.1E+01	3

(FOR ALPHA/S(1) = 4.26E-02) PRUNS = 0.0000 PUNCOR = 0.0000 0.0000 0.0000 0.0000 0.0000

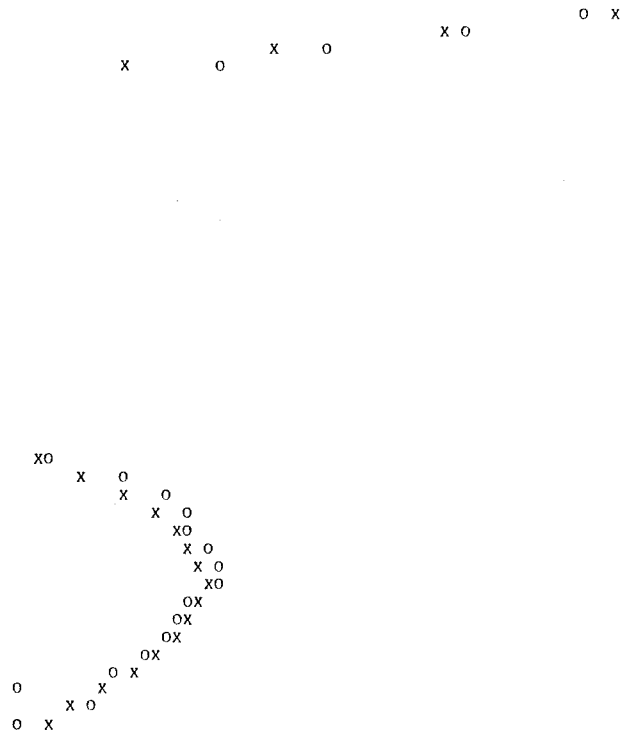
WEIGHTED RESIDUALS (ALPHA/S(1)= 5.75E-03) MAX=U= 2.5E-01 MIN=L=-3.1E-01 (PRUNS= 0.0000) PUNCOR= 0.0818 0.6547 0.2590 0.7581 0.2042



MAR 84 Page 16

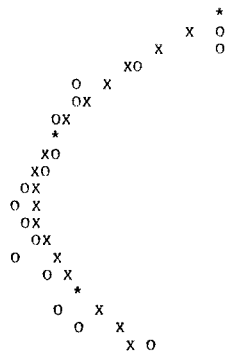
PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
1.610E+00	1.60E-02
1.137E+00	1.70E-02
6.929E-01	1.80E-02
2.819E-01	1.90E-02
-9.157E-02	2.00E-02
-4.241E-01	2.10E-02
-7.134E-01	2.20E-02
-9.576E-01	2.30E-02
-1.156E+00	2.40E-02
-1.309E+00	2.50E-02
-1.418E+00	2.60E-02
-1.483E+00	2.70E-02
-1.509E+00	2.80E-02
-1.496E+00	2.90E-02
-1.450E+00	3.00E-02
-1.374E+00	3.10E-02
-1.273E+00	3.20E-02
-1.150E+00	3.30E-02
-1.011E+00	3.40E-02
-8.608E-01	3.50E-02
-7.031E-01	3.60E-02
-5.427E-01	3.70E-02
-3.838E-01	3.80E-02
-2.302E-01	3.90E-02
-8.540E-02	4.00E-02
4.753E-02	4.10E-02
1.661E-01	4.20E-02
2.682E-01	4.30E-02
3.525E-01	4.40E-02
4.178E-01	4.50E-02
4.638E-01	4.60E-02
4.905E-01	4.70E-02
4.984E-01	4.80E-02
4.884E-01	4.90E-02
4.620E-01	5.00E-02
4.207E-01	5.10E-02
3.666E-01	5.20E-02
3.017E-01	5.30E-02
2.285E-01	5.40E-02
1.492E-01	5.50E-02
6.641E-02	5.60E-02



MAR 84 Page 17

-1.764E-02	5.70E-02
-1.006E-01	5.80E-02
-1.804E-01	5.90E-02
-2.552E-01	6.00E-02
-3.231E-01	6.10E-02
-3.829E-01	6.20E-02
-4.333E-01	6.30E-02
-4.737E-01	6.40E-02
-5.034E-01	6.50E-02
-5.224E-01	6.60E-02
-5.306E-01	6.70E-02
-5.286E-01	6.80E-02
-5.170E-01	6.90E-02
-4.965E-01	7.00E-02
-4.684E-01	7.10E-02
-4.337E-01	7.20E-02
-3.938E-01	7.30E-02
-3.500E-01	7.40E-02
-3.038E-01	7.50E-02
-2.563E-01	7.60E-02



ERRFIT = 0.00E+00

SQUARE ROOTS OF LEAST SQUARES WEIGHTS

7.5135E-01	6.2670E-01	4.4000E-01	1.9549E-01	6.4613E-02	2.8727E-01	4.5037E-01	5.6068E-01	6.3294E-01	6.7935E-01
7.0799E-01	7.2378E-01	7.2956E-01	7.2678E-01	7.1596E-01	6.9694E-01	6.6900E-01	6.3103E-01	5.8173E-01	5.1995E-01
4.4518E-01	3.5826E-01	2.6188E-01	1.6064E-01	6.0279E-02	3.3592E-02	1.1664E-01	1.8635E-01	2.4184E-01	2.8333E-01
3.1162E-01	3.2767E-01	3.3236E-01	3.2644E-01	3.1052E-01	2.8514E-01	2.5092E-01	2.0866E-01	1.5950E-01	1.0495E-01
4.6905E-02	1.2473E-02	7.0978E-02	1.2657E-01	1.7756E-01	2.2273E-01	2.6132E-01	2.9296E-01	3.1759E-01	3.3535E-01
3.4648E-01	3.5130E-01	3.5013E-01	3.4333E-01	3.3129E-01	3.1441E-01	2.9321E-01	2.6827E-01	2.4027E-01	2.1000E-01
1.7833E-01									

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
0.0000E+00	0.0000D+00	1.60D-02	0.0000D+00	1.60D-02	4.459D-03
1.5000E+00	2.1845D-01	5.70D-02	1.4082D+01	1.60D-02	1.486D-03
3.0000E+00	1.7200D-01	5.70D-02	1.3842D+01	1.60D-02	1.115D-03
4.5000E+00	3.1653D-01	5.70D-02	4.0341D+01	1.60D-02	1.115D-03
6.0000E+00	-1.6688D+00	7.30D-02	2.5807D+01	1.60D-02	1.115D-03
7.5000E+00	-1.0779D+01	6.90D-02	6.1101D+01	1.60D-02	1.115D-03
9.0000E+00	-7.9936D+00	6.70D-02	3.4227D+01	1.60D-02	1.115D-03
1.0500E+01	-1.6062D+01	6.50D-02	7.3387D+01	1.60D-02	1.115D-03
1.2000E+01	-9.8614D+00	4.80D-02	3.7840D+01	1.60D-02	1.115D-03
1.3500E+01	-2.2124D+01	4.70D-02	7.5190D+01	1.60D-02	1.115D-03
1.5000E+01	-1.7618D+01	3.40D-02	3.5929D+01	1.60D-02	1.115D-03
1.6500E+01	-4.8286D+01	3.20D-02	6.5705D+01	1.60D-02	1.115D-03
1.8000E+01	-3.0027D+01	3.10D-02	2.8418D+01	1.60D-02	1.115D-03
1.9500E+01	-6.9791D+01	3.00D-02	4.5439D+01	1.60D-02	1.115D-03
2.1000E+01	-3.8623D+01	2.90D-02	1.5889D+01	1.60D-02	1.115D-03
2.2500E+01	-8.2421D+01	2.80D-02	2.7592D+01	4.90D-02	1.115D-03
2.4000E+01	-4.2830D+01	2.60D-02	1.4791D+01	4.70D-02	1.115D-03
2.5500E+01	-8.6460D+01	2.60D-02	2.8134D+01	4.60D-02	1.115D-03
2.7000E+01	-4.2707D+01	2.50D-02	1.3529D+01	3.60D-02	1.115D-03
2.8500E+01	-8.1925D+01	2.40D-02	4.0392D+01	3.50D-02	1.115D-03
3.0000E+01	-3.7960D+01	1.70D-02	2.6855D+01	3.40D-02	1.115D-03
3.1500E+01	-9.2576D+01	1.60D-02	6.6256D+01	3.40D-02	1.115D-03
3.3000E+01	-5.4230D+01	1.60D-02	3.8675D+01	3.30D-02	1.115D-03
3.4500E+01	-1.2234D+02	1.60D-02	8.6772D+01	3.20D-02	1.115D-03
3.6000E+01	-6.6878D+01	1.60D-02	4.7312D+01	3.00D-02	1.115D-03
3.7500E+01	-1.4233D+02	1.60D-02	1.0111D+02	3.00D-02	1.115D-03
3.9000E+01	-9.2327D+01	1.60D-02	6.6537D+01	2.90D-02	1.115D-03
4.0500E+01	-5.6134D+01	1.60D-02	4.1538D+01	2.80D-02	1.115D-03

SCALE FACTOR FOR ALPHA = 6.279E+03

0 UNREGULARIZED VARIABLES

SINGULAR VALUES

5.698E+00	1.935E+00	5.894E-01	1.808E-01	7.843E-02	6.469E-02	1.649E-02	1.885E-03	1.429E-04	9.491E-06
3.862E-07	1.428E-08	3.526E-09	2.241E-09	2.097E-09	1.878E-09	1.658E-09	1.427E-09	1.053E-09	7.894E-10
6.237E-10	5.829E-10	4.733E-10	3.573E-10	1.684E-10	1.137E-10	7.652E-18			

TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 1.06E-15	1.86E-16	1.91987E-02	1.91987E-02	1.921E-02	9.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA
-1.000E-02	1.6D-19	0.00E+00X
7.275E-02	3.3D-03	1.50E+00
-1.000E-02	8.2D-19	3.00E+00X
-1.000E-02	1.2D-18	4.50E+00X
-1.000E-02	3.2D-18	6.00E+00X
-1.000E-02	1.1D-19	7.50E+00X
-1.000E-02	1.9D-18	9.00E+00X
-1.000E-02	2.8D-18	1.05E+01X
6.442E-02	1.5D-02	1.20E+01
1.827E-02	8.9D-03	1.35E+01
-1.000E-02	9.8D-19	1.50E+01X
-1.000E-02	5.0D-19	1.65E+01X
-1.000E-02	1.1D-18	1.80E+01X
-1.000E-02	6.4D-19	1.95E+01X
-1.000E-02	1.5D-18	2.10E+01X
4.845E-02	1.7D-02	2.25E+01
-7.487E-04	4.2D-02	2.40E+01
-1.000E-02	1.1D-17	2.55E+01X
-1.000E-02	5.2D-18	2.70E+01X
-1.000E-02	5.6D-19	2.85E+01X
-7.226E-03	4.2D-02	3.00E+01
3.081E-02	1.8D-02	3.15E+01
-1.000E-02	9.4D-18	3.30E+01X
-1.000E-02	4.1D-18	3.45E+01X
-1.000E-02	8.2D-18	3.60E+01X
5.828E-03	5.9D-03	3.75E+01
4.115E-05	6.0D-03	3.90E+01
0.000E+00	0.0D+00	4.05E+01

MAR 84 Page 18

PEAK 1 GOES FROM 0.000E+00 TO 1.050E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	5.0500 X (10** -2)	1.3E+01			
1	-4.1175 X (10** -1)	2.4E+00	-8.1535E+00	1.5E+01	1
2	-4.6676 X (10** 0)	3.2E-01	1.1336E+01	2.7E+00	2
3	-4.2641 X (10** 1)	5.2E-02	9.1356E+00	3.7E-01	3

PEAK 2 GOES FROM 1.200E+01 TO 2.100E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	3.0948 X (10** -2)	9.7E+00			
1	6.1757 X (10** -3)	1.0E+03	1.9955E-01	1.0E+03	1
2	-7.0161 X (10** 0)	1.6E+01	-1.1361E+03	1.0E+03	2
3	-2.2163 X (10** 2)	8.2E+00	3.1588E+01	2.4E+01	3

PEAK 3 GOES FROM 2.250E+01 TO 2.850E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	4.6157 X (10** -2)	1.6E+01			
1	8.1242 X (10** -1)	2.8E+01	1.7601E+01	4.3E+01	1
2	1.2087 X (10** 1)	5.4E+01	1.4878E+01	8.2E+01	2
3	1.0203 X (10** 2)	1.8E+02	8.4411E+00	2.3E+02	3

PEAK 4 GOES FROM 3.000E+01 TO 4.050E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	2.6110 X (10** -2)	3.6E+01			
1	7.8362 X (10** -1)	3.2E+01	3.0012E+01	6.8E+01	1
2	2.3462 X (10** 1)	2.7E+01	2.9940E+01	5.9E+01	2
3	7.0167 X (10** 2)	2.3E+01	2.9907E+01	5.1E+01	3

MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 1.3E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	1.5371 X (10** -1)	9.0E+00			
1	1.1905 X (10** 0)	2.9E+01	7.7446E+00	3.8E+01	1
2	2.3866 X (10** 1)	3.9E+01	2.0047E+01	6.8E+01	2
3	5.3943 X (10** 2)	4.6E+01	2.2603E+01	8.5E+01	3

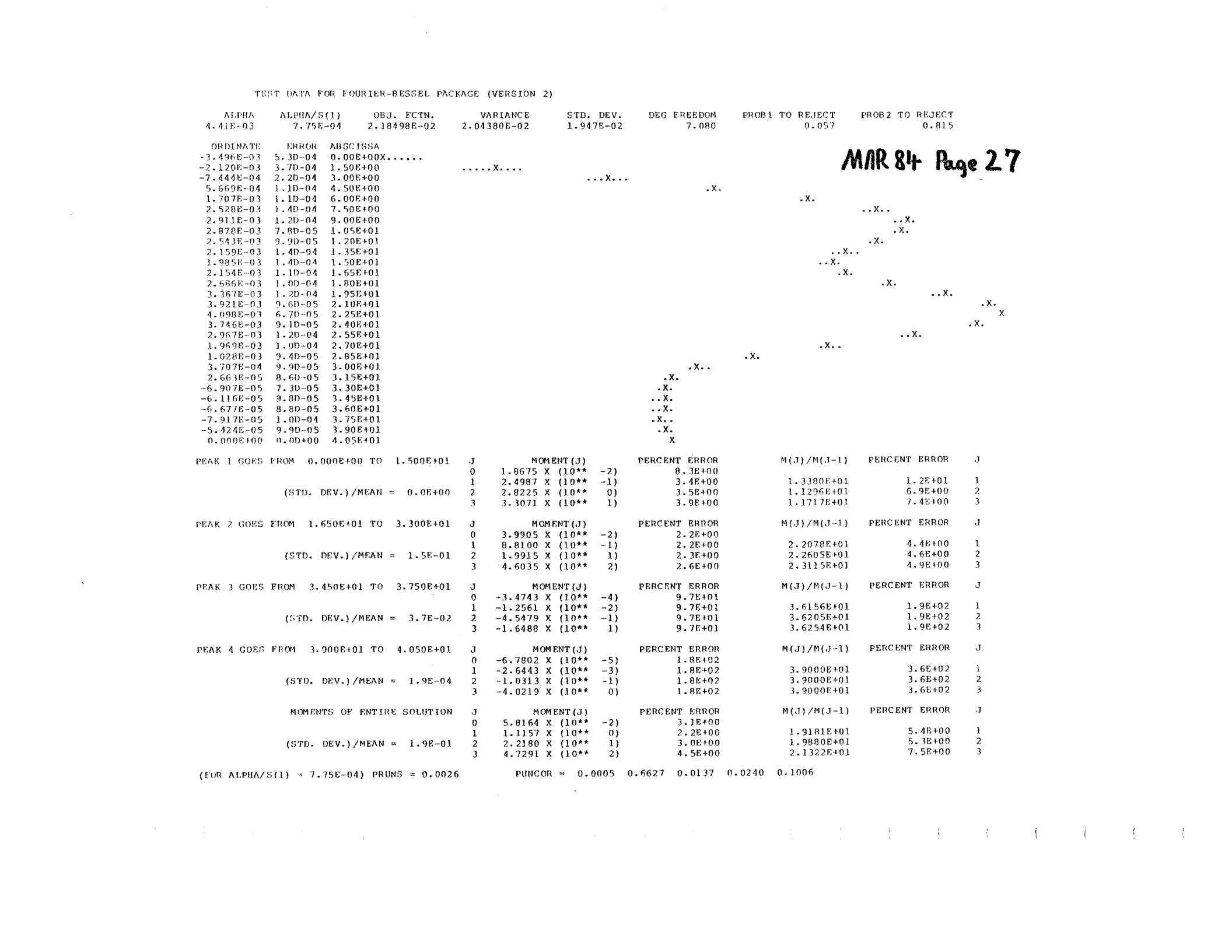
(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.0363 PUNCOR = 0.0033 0.2130 0.0007 0.0218 0.2800

TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
4.41E-03	7.75E-04	2.18498E-02	2.04380E-02	1.947E-02	7.080	0.057	0.815

MAR 84 Page 27

ORDINATE	ERROR	ABSCISSA
-3.496E-03	5.3D-04	0.00E+00
-2.120E-03	3.7D-04	1.50E+00
-7.444E-04	2.2D-04	3.00E+00
5.669E-04	1.1D-04	4.50E+00
1.707E-03	1.1D-04	6.00E+00
2.528E-03	1.4D-04	7.50E+00
2.911E-03	1.2D-04	9.00E+00
2.878E-03	7.8D-05	1.05E+01
2.543E-03	9.9D-05	1.20E+01
2.159E-03	1.4D-04	1.35E+01
1.985E-03	1.4D-04	1.50E+01
2.154E-03	1.1D-04	1.65E+01
2.686E-03	1.0D-04	1.80E+01
3.367E-03	1.2D-04	1.95E+01
3.921E-03	9.6D-05	2.10E+01
4.098E-03	6.7D-05	2.25E+01
3.746E-03	9.1D-05	2.40E+01
2.967E-03	1.2D-04	2.55E+01
1.969E-03	1.0D-04	2.70E+01
1.028E-03	9.4D-05	2.85E+01
3.707E-04	9.9D-05	3.00E+01
2.663E-05	8.6D-05	3.15E+01
-6.907E-05	7.3D-05	3.30E+01
-6.116E-05	9.8D-05	3.45E+01
-6.677E-05	8.8D-05	3.60E+01
-7.917E-05	1.0D-04	3.75E+01
-5.424E-05	9.9D-05	3.90E+01
0.000E+00	0.0D+00	4.05E+01

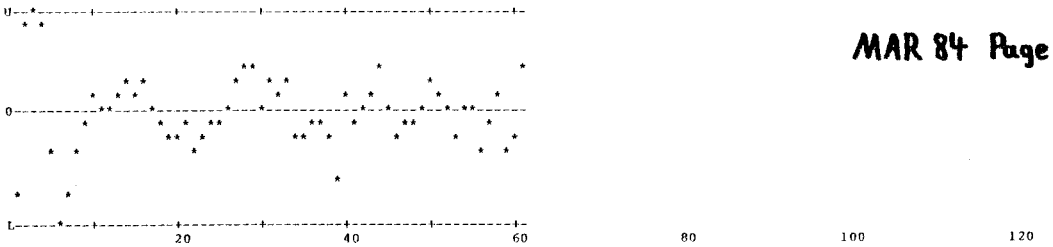


	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
PEAK 1 GOES FROM 0.000E+00 TO 1.500E+01	0	1.8675 X (10** -2)	8.3E+00			
	1	2.4987 X (10** -1)	3.4E+00	1.3380E+01	1.2E+01	1
(STD. DEV.)/MEAN = 0.0E+00	2	2.8225 X (10** 0)	3.5E+00	1.1296E+01	6.9E+00	2
	3	3.3071 X (10** 1)	3.9E+00	1.1717E+01	7.4E+00	3
PEAK 2 GOES FROM 1.650E+01 TO 3.300E+01	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
	0	3.9905 X (10** -2)	2.2E+00			
	1	8.8100 X (10** -1)	2.2E+00	2.2078E+01	4.4E+00	1
(STD. DEV.)/MEAN = 1.5E-01	2	1.9915 X (10** 1)	2.3E+00	2.2605E+01	4.6E+00	2
	3	4.6035 X (10** 2)	2.6E+00	2.3115E+01	4.9E+00	3
PEAK 3 GOES FROM 3.450E+01 TO 3.750E+01	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
	0	-3.4743 X (10** -4)	9.7E+01			
	1	-1.2561 X (10** -2)	9.7E+01	3.6156E+01	1.9E+02	1
(STD. DEV.)/MEAN = 3.7E-02	2	-4.5479 X (10** -1)	9.7E+01	3.6205E+01	1.9E+02	2
	3	-1.6488 X (10** 1)	9.7E+01	3.6254E+01	1.9E+02	3
PEAK 4 GOES FROM 3.900E+01 TO 4.050E+01	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
	0	-6.7802 X (10** -5)	1.8E+02			
	1	-2.6443 X (10** -3)	1.8E+02	3.9000E+01	3.6E+02	1
(STD. DEV.)/MEAN = 1.9E-04	2	-1.0313 X (10** -1)	1.8E+02	3.9000E+01	3.6E+02	2
	3	-4.0219 X (10** 0)	1.8E+02	3.9000E+01	3.6E+02	3
MOMENTS OF ENTIRE SOLUTION	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
	0	5.8164 X (10** -2)	3.1E+00			
	1	1.1157 X (10** 0)	2.2E+00	1.9181E+01	5.4E+00	1
(STD. DEV.)/MEAN = 1.9E-01	2	2.2180 X (10** 1)	3.0E+00	1.9880E+01	5.3E+00	2
	3	4.7291 X (10** 2)	4.5E+00	2.1322E+01	7.5E+00	3

(FOR ALPHA/S(1) = 7.75E-04) PRUNS = 0.0026 PUNCOR = 0.0005 0.6627 0.0137 0.0240 0.1006

CONTIN 2DP (MAR 84) (FBS-1) TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2) CHOSEN SOLUTION

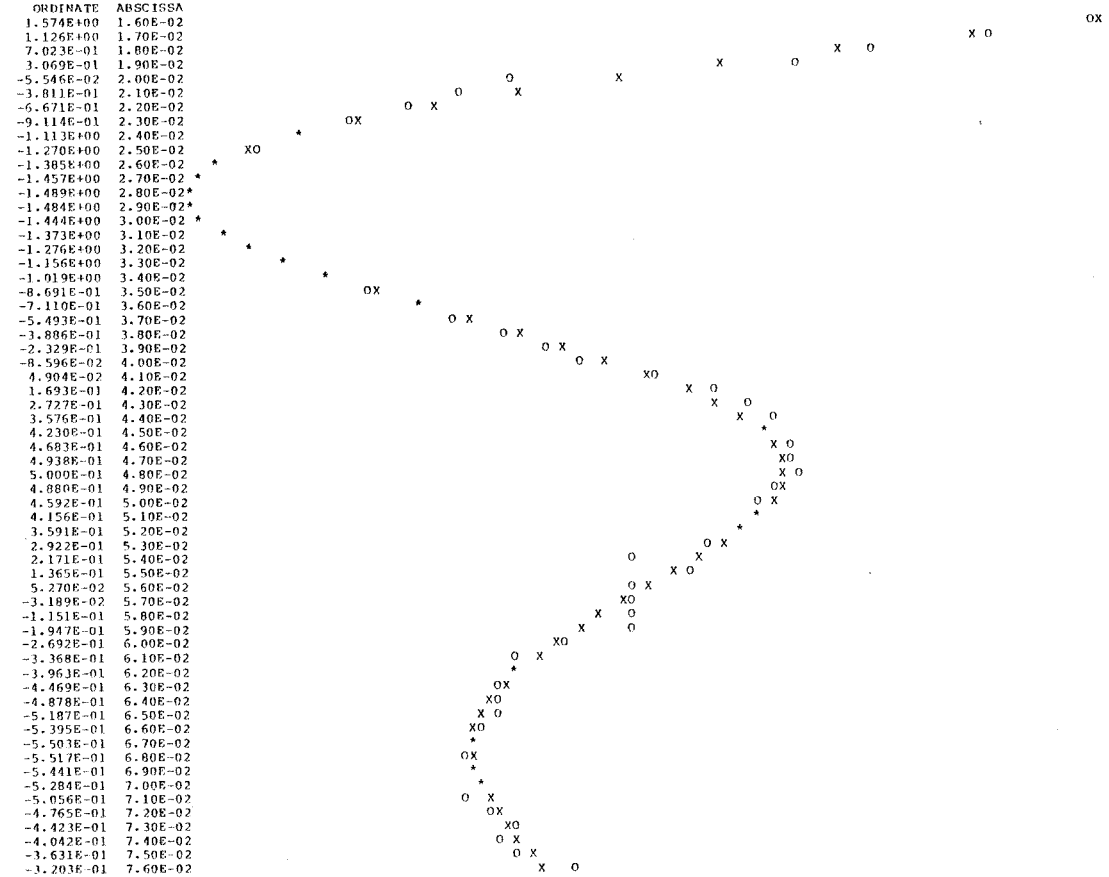
WEIGHTED RESIDUALS (ALPHA/S(1)= 7.75E-04) MAX=U= 4.9E-02 MIN=L=-5.3E-02 (PRUNS= 0.0026) PUNCOR= 0.0005 0.6627 0.0137 0.0240 0.1006



MAR 84 Page 30

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA
1.574E+00	1.60E-02
1.126E+00	1.70E-02
7.023E-01	1.80E-02
3.069E-01	1.90E-02
-5.546E-02	2.00E-02
-3.811E-01	2.10E-02
-6.671E-01	2.20E-02
-9.114E-01	2.30E-02
-1.113E+00	2.40E-02
-1.270E+00	2.50E-02
-1.385E+00	2.60E-02
-1.457E+00	2.70E-02
-1.489E+00	2.80E-02
-1.484E+00	2.90E-02
-1.444E+00	3.00E-02
-1.373E+00	3.10E-02
-1.276E+00	3.20E-02
-1.156E+00	3.30E-02
-1.019E+00	3.40E-02
-8.691E-01	3.50E-02
-7.110E-01	3.60E-02
-5.493E-01	3.70E-02
-3.886E-01	3.80E-02
-2.329E-01	3.90E-02
-8.596E-02	4.00E-02
4.904E-02	4.10E-02
1.693E-01	4.20E-02
2.727E-01	4.30E-02
3.576E-01	4.40E-02
4.230E-01	4.50E-02
4.683E-01	4.60E-02
4.938E-01	4.70E-02
5.000E-01	4.80E-02
4.880E-01	4.90E-02
4.592E-01	5.00E-02
4.156E-01	5.10E-02
3.591E-01	5.20E-02
2.922E-01	5.30E-02
2.171E-01	5.40E-02
1.365E-01	5.50E-02
5.270E-02	5.60E-02
-3.189E-02	5.70E-02
-1.151E-01	5.80E-02
-1.947E-01	5.90E-02
-2.692E-01	6.00E-02
-3.368E-01	6.10E-02
-3.963E-01	6.20E-02
-4.469E-01	6.30E-02
-4.878E-01	6.40E-02
-5.187E-01	6.50E-02
-5.395E-01	6.60E-02
-5.503E-01	6.70E-02
-5.517E-01	6.80E-02
-5.441E-01	6.90E-02
-5.284E-01	7.00E-02
-5.056E-01	7.10E-02
-4.765E-01	7.20E-02
-4.423E-01	7.30E-02
-4.042E-01	7.40E-02
-3.631E-01	7.50E-02
-3.203E-01	7.60E-02

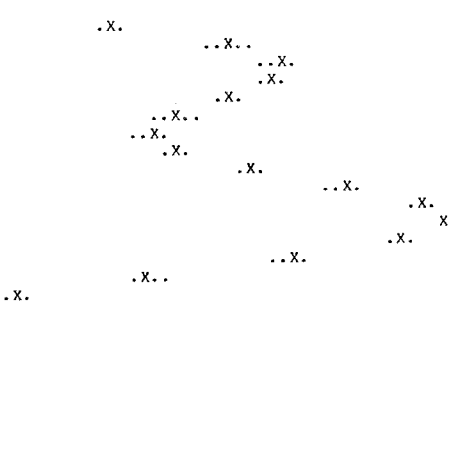


TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
4.41E-03	7.75E-04	2.18498E-02	2.04380E-02	1.947E-02	7.080	0.057	0.815

MAR 84 Page 32

ORDINATE	ERROR	ABSCISSA
-3.496E-03	5.3D-04	0.00E+00
-2.120E-03	3.7D-04	1.50E+00
-7.444E-04	2.2D-04	3.00E+00
5.669E-04	1.1D-04	4.50E+00
1.707E-03	1.1D-04	6.00E+00
2.528E-03	1.4D-04	7.50E+00
2.911E-03	1.2D-04	9.00E+00
2.878E-03	7.8D-05	1.05E+01
2.543E-03	9.9D-05	1.20E+01
2.159E-03	1.4D-04	1.35E+01
1.985E-03	1.4D-04	1.50E+01
2.154E-03	1.1D-04	1.65E+01
2.686E-03	1.0D-04	1.80E+01
3.367E-03	1.2D-04	1.95E+01
3.921E-03	9.6D-05	2.10E+01
4.098E-03	6.7D-05	2.25E+01
3.746E-03	9.1D-05	2.40E+01
2.967E-03	1.2D-04	2.55E+01
1.969E-03	1.0D-04	2.70E+01
1.028E-03	9.4D-05	2.85E+01
3.707E-04	9.9D-05	3.00E+01
2.663E-05	8.6D-05	3.15E+01
-6.907E-05	7.3D-05	3.30E+01
-6.116E-05	9.8D-05	3.45E+01
-6.677E-05	8.8D-05	3.60E+01
-7.917E-05	1.0D-04	3.75E+01
-5.424E-05	9.9D-05	3.90E+01
0.000E+00	0.0D+00	4.05E+01



PEAK 1 GOES FROM 0.000E+00 TO 1.500E+01

(STD. DEV.)/MEAN = 0.0E+00

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	1.8675 X (10** -2)	8.3E+00			
1	2.4987 X (10** -1)	3.4E+00	1.3380E+01	1.2E+01	1
2	2.8225 X (10** 0)	3.5E+00	1.1296E+01	6.9E+00	2
3	3.3071 X (10** 1)	3.9E+00	1.1717E+01	7.4E+00	3

PEAK 2 GOES FROM 1.650E+01 TO 3.300E+01

(STD. DEV.)/MEAN = 1.5E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	3.9905 X (10** -2)	2.2E+00			
1	8.8100 X (10** -1)	2.2E+00	2.2078E+01	4.4E+00	1
2	1.9915 X (10** 1)	2.3E+00	2.2605E+01	4.6E+00	2
3	4.6035 X (10** 2)	2.6E+00	2.3115E+01	4.9E+00	3

PEAK 3 GOES FROM 3.450E+01 TO 3.750E+01

(STD. DEV.)/MEAN = 3.7E-02

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	-3.4743 X (10** -4)	9.7E+01			
1	-1.2561 X (10** -2)	9.7E+01	3.6156E+01	1.9E+02	1
2	-4.5479 X (10** -1)	9.7E+01	3.6205E+01	1.9E+02	2
3	-1.6488 X (10** 1)	9.7E+01	3.6254E+01	1.9E+02	3

PEAK 4 GOES FROM 3.900E+01 TO 4.050E+01

(STD. DEV.)/MEAN = 1.9E-04

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	-6.7802 X (10** -5)	1.8E+02			
1	-2.6443 X (10** -3)	1.8E+02	3.9000E+01	3.6E+02	1
2	-1.0313 X (10** -1)	1.8E+02	3.9000E+01	3.6E+02	2
3	-4.0219 X (10** 0)	1.8E+02	3.9000E+01	3.6E+02	3

MOMENTS OF ENTIRE SOLUTION

(STD. DEV.)/MEAN = 1.9E-01

J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
0	5.8164 X (10** -2)	3.1E+00			
1	1.1157 X (10** 0)	2.2E+00	1.9181E+01	5.4E+00	1
2	2.2180 X (10** 1)	3.0E+00	1.9880E+01	5.3E+00	2
3	4.7291 X (10** 2)	4.5E+00	2.1322E+01	7.5E+00	3

MAR 84 Page 1

```
CONTIN - VERSION 2DP (MAR 1984) ( CD-1  PACK)       TEST DATA SET 1 - FOR CD PACKAGE

REFERENCES - S.W. PROVENCHER (1982) COMPUT. PHYS. COMMUN., VOL. 27, PAGES 213-227, 229-242.
                            (1984) EMBL TECHNICAL REPORT DA07 (EUROPEAN MOLECULAR BIOLOGY LABORATORY, HEIDELBERG, F.R. OF GERMANY)


                   INPUT DATA FOR CHANGES TO COMMON VARIABLES

IFORMY     0     0.00000E+00
(7F9.0)

LAST       0    -1.00000E+00

END        0     0.00000E+00
NSTEND    26     1.90000E+02     2.40000E+02


                                      FINAL VALUES OF CONTROL VARIABLES
DFMIN  = 3.00000E+00
SRMIN  = 1.00000E-02
ALPST  = 0.00000E+00 0.00000E+00
GMNMX  = 1.00000E+00 1.60000E+01
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+00 1.00000E-03 5.00000E+02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
IGRID  =          1
IQUAD  =          1
IUNIT  =         -1
IWT    =          1
LINEPG =         60
MIOERR =          5
MPKMOM =          0
MQPITR =         35
NEQ    =          0
NERFIT =          0
NG     =         16
NINTT  =          1
NLINF  =          0
NORDER =         -1
ICRIT  =          1          1
IFORMT = (5E15.6)
IFORMW = (5E15.6)
IFORMY = (7F9.0)
IPLFIT =          2          2
IPLRES =          2          2
```

```
IPRINT =          2          3
IUSER  =          0          0          0          0          0          0          0          0          0          0
                  0          0          0          0          0          4          7          0          0          0
                  0          0          0          0          0          0          0          0          0          0
                  0          0          0          0          0          0          0          0          0          0
                  0          0          0          0          0          0          0          0          0          0
IUSROU =          3          3
LSIGN  =          0          0          0          0          0          0          0          0          0          0
                  0          0          0          0          0          0
MOMNMX =          0          0
NENDZ  =          0          0
NFLAT  =          0          0          0          0          0          0          0          0
NNSGN  =          0          0
NQPROG =          6          6
NSGN   =          0          0          0          0
DOCHOS =          T
DOMOM  =          F
DOUSIN =          T
DOUSNQ =          T
LAST   =          F
NEWPG1 =          F
NONNEG =          F
ONLY1  =          T
PRWT   =          T
PRY    =          T
SIMULA =          F
LUSER  =          F          F          F          F          F          F          F          F          F          F
                  F          F          F          F          F          F          F          F          F          F
                  F          F          F          F          F          F          F          F          F          F
```

MAR 84 Page 2

T	Y	T	Y	T	Y	T	Y	T	Y
1.900E+02	4.68320E+04	1.920E+02	4.44010E+04	1.940E+02	3.59750E+04	1.960E+02	2.04180E+04	1.980E+02	2.59200E+03
2.000E+02	-6.48200E+03	2.020E+02	-1.97700E+04	2.040E+02	-2.62520E+04	2.060E+02	-3.04650E+04	2.080E+02	-2.80340E+04
2.100E+02	-2.49550E+04	2.120E+02	-2.33350E+04	2.140E+02	-2.30110E+04	2.160E+02	-2.28490E+04	2.180E+02	-2.31730E+04
2.200E+02	-2.31730E+04	2.220E+02	-2.28490E+04	2.240E+02	-1.99320E+04	2.260E+02	-1.92840E+04	2.280E+02	-1.57190E+04
2.300E+02	-1.19910E+04	2.320E+02	-8.75000E+03	2.340E+02	-5.99500E+03	2.360E+02	-3.56500E+03	2.380E+02	-2.26800E+03
2.400E+02	-1.45800E+03	0.000E+00	1.00000E+00						

PRECIS = 1.86D-16 SRANGE = 1.00E+35 RANGE = 1.00D+35

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
1.0000E+00	-2.4876D+04	2.22D+02	5.0000D+05	0.00D+00	1.359D-06
2.0000E+00	-1.3387D+04	2.08D+02	5.0000D+05	0.00D+00	1.359D-06
3.0000E+00	-1.1077D+04	2.10D+02	5.0000D+05	0.00D+00	1.359D-06
4.0000E+00	-1.2588D+04	2.10D+02	5.0000D+05	0.00D+00	1.359D-06
5.0000E+00	-1.3227D+04	2.22D+02	5.0000D+05	0.00D+00	1.359D-06
6.0000E+00	-9.7595D+03	2.02D+02	5.0000D+05	0.00D+00	1.359D-06
7.0000E+00	-6.6914D+03	2.24D+02	5.0000D+05	0.00D+00	1.359D-06
8.0000E+00	-1.2232D+04	2.22D+02	5.0000D+05	0.00D+00	1.359D-06
9.0000E+00	-1.2404D+04	2.00D+02	5.0000D+05	0.00D+00	1.359D-06
1.0000E+01	-1.1117D+04	2.08D+02	5.0000D+05	0.00D+00	1.359D-06
1.1000E+01	-1.3576D+04	2.10D+02	5.0000D+05	0.00D+00	1.359D-06
1.2000E+01	-1.4514D+04	2.22D+02	5.0000D+05	0.00D+00	1.359D-06
1.3000E+01	-9.9252D+03	2.12D+02	5.0000D+05	0.00D+00	1.359D-06
1.4000E+01	-1.8460D+04	2.04D+02	5.0000D+05	0.00D+00	1.359D-06
1.5000E+01	-1.4012D+04	2.10D+02	5.0000D+05	0.00D+00	1.359D-06
1.6000E+01	-1.1052D+04	2.12D+02	5.0000D+05	0.00D+00	1.359D-06

SCALE FACTOR FOR ALPHA = 1.177E+07

0 UNREGULARIZED VARIABLES

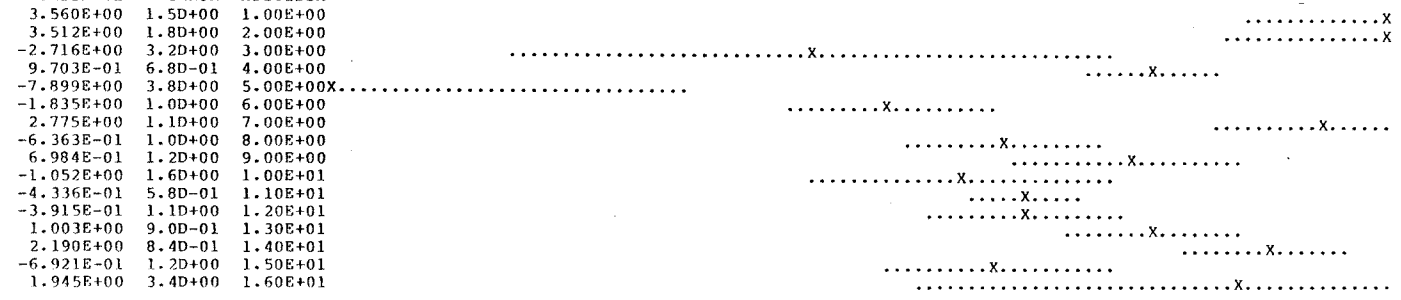
SINGULAR VALUES

1.707E-01	1.105E-02	4.685E-03	1.856E-03	1.272E-03	8.837E-04	6.458E-04	2.453E-04	2.366E-04	1.524E-04
1.298E-04	5.636E-05	3.900E-05	3.319E-05	1.458E-05	1.123E-05				

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 3.18E-17	1.86E-16	5.65587E+06	5.65587E+06	7.171E+02	16.000	0.000	1.000

ORDINATE	ERROR	ABSCISSA
3.560E+00	1.5D+00	1.00E+00
3.512E+00	1.8D+00	2.00E+00
-2.716E+00	3.2D+00	3.00E+00
9.703E-01	6.8D-01	4.00E+00
-7.899E+00	3.8D+00	5.00E+00
-1.835E+00	1.0D+00	6.00E+00
2.775E+00	1.1D+00	7.00E+00
-6.363E-01	1.0D+00	8.00E+00
6.984E-01	1.2D+00	9.00E+00
-1.052E+00	1.6D+00	1.00E+01
-4.336E-01	5.8D-01	1.10E+01
-3.915E-01	1.1D+00	1.20E+01
1.003E+00	9.0D-01	1.30E+01
2.190E+00	8.4D-01	1.40E+01
-6.921E-01	1.2D+00	1.50E+01
1.945E+00	3.4D+00	1.60E+01



	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.44	0.24	0.33	1.000
STANDARD ERROR	2.3E-01	2.3E-01	4.0E-01	

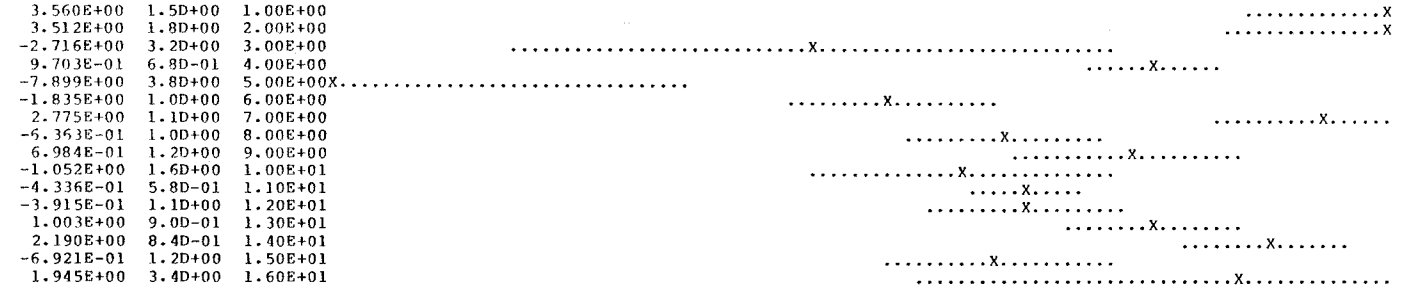
MAR 84 Page 3

(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.9990 PUNCOR = 0.0001 0.0416 0.0424 0.0867 0.2655

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 2.23E-14	1.31E-13	5.65587E+06	5.65587E+06	7.171E+02	16.000	0.000	1.000

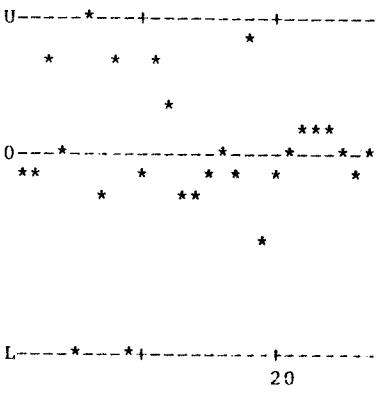
ORDINATE	ERROR	ABSCISSA
3.560E+00	1.5D+00	1.00E+00
3.512E+00	1.8D+00	2.00E+00
-2.716E+00	3.2D+00	3.00E+00
9.703E-01	6.8D-01	4.00E+00
-7.899E+00	3.8D+00	5.00E+00
-1.835E+00	1.0D+00	6.00E+00
2.775E+00	1.1D+00	7.00E+00
-6.363E-01	1.0D+00	8.00E+00
6.984E-01	1.2D+00	9.00E+00
-1.052E+00	1.6D+00	1.00E+01
-4.336E-01	5.8D-01	1.10E+01
-3.915E-01	1.1D+00	1.20E+01
1.003E+00	9.0D-01	1.30E+01
2.190E+00	8.4D-01	1.40E+01
-6.921E-01	1.2D+00	1.50E+01
1.945E+00	3.4D+00	1.60E+01



	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.44	0.24	0.33	1.000
STANDARD ERROR	2.3E-01	2.3E-01	4.0E-01	

(FOR ALPHA/S(1) = 1.31E-13) PRUNS = 0.9990 PUNCOR = 0.0001 0.0416 0.0424 0.0867 0.2655

WEIGHTED RESIDUALS (ALPHA/S(1)= 7.48E-04) MAX=U= 1.4E+03 MIN=L=-1.9E+03 (PRUNS= 0.7862) PUNCOR= 0.0444 0.6070 0.2335 0.1838 0.5010



MAR 84 Page 9

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

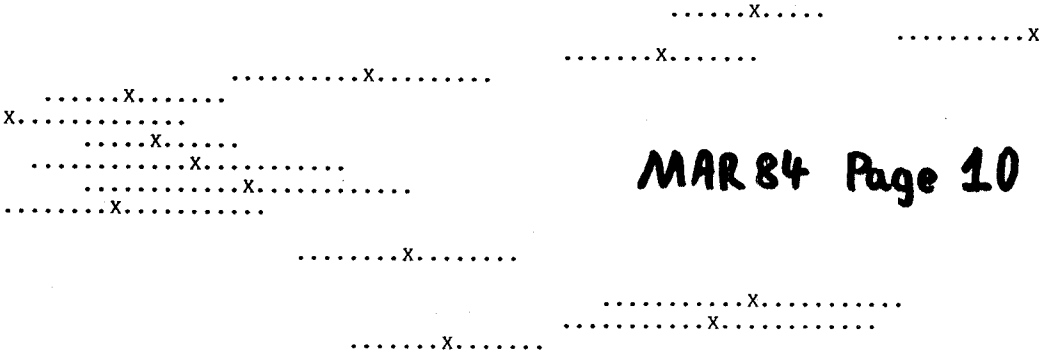
ORDINATE	ABSCISSA
4.704E+04	1.90E+02
4.447E+04	1.92E+02
3.508E+04	1.94E+02
2.022E+04	1.96E+02
4.460E+03	1.98E+02
-7.884E+03	2.00E+02
-1.948E+04	2.02E+02
-2.732E+04	2.04E+02
-2.869E+04	2.06E+02
-2.787E+04	2.08E+02
-2.592E+04	2.10E+02
-2.382E+04	2.12E+02
-2.266E+04	2.14E+02
-2.253E+04	2.16E+02
-2.302E+04	2.18E+02
-2.320E+04	2.20E+02
-2.267E+04	2.22E+02
-2.106E+04	2.24E+02
-1.859E+04	2.26E+02
-1.555E+04	2.28E+02
-1.209E+04	2.30E+02
-9.000E+03	2.32E+02
-6.210E+03	2.34E+02
-3.919E+03	2.36E+02
-2.327E+03	2.38E+02
-1.356E+03	2.40E+02
1.000E+00	0.00E+00

CONTIN VERSION 2DP (MAR 1984) (CD-1 PACKAGE) ++++++++++++++++++++++++++++++++ CHOSEN SOLUTION ++++++++++++++++++++++++++++++++

TEST DATA SET 1 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.28E-04	7.48E-04	2.17297E+07	1.42189E+07	9.123E+02	9.917	0.515	0.930

ORDINATE	ERROR	ABSCISSA
5.844E-01	9.6D-02	1.00E+00
9.564E-01	1.8D-01	2.00E+00
4.609E-01	1.2D-01	3.00E+00
8.559E-02	1.6D-01	4.00E+00
-2.183E-01	1.1D-01	5.00E+00
-3.763E-01	2.3D-01	6.00E+00
-1.783E-01	9.8D-02	7.00E+00
-1.383E-01	2.0D-01	8.00E+00
-6.425E-02	2.0D-01	9.00E+00
-2.299E-01	1.8D-01	1.00E+01
-5.898E-01	1.9D-01	1.10E+01
1.463E-01	1.4D-01	1.20E+01
-7.592E-01	1.6D-01	1.30E+01
5.829E-01	1.9D-01	1.40E+01
5.446E-01	2.0D-01	1.50E+01
1.934E-01	1.2D-01	1.60E+01



	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.75	0.10	0.14	1.000
STANDARD ERROR	3.9E-02	7.1E-02	6.5E-02	

MAR 84 Page 10

```
CONTIN - VERSION 2DP (MAR 1984) ( CD-1  PACK)        TEST DATA SET 2 - FOR CD PACKAGE

REFERENCES - S.W. PROVENCHER (1982) COMPUT. PHYS. COMMUN., VOL. 27, PAGES 213-227, 229-242.
                             (1984) EMBL TECHNICAL REPORT DA07 (EUROPEAN MOLECULAR BIOLOGY LABORATORY, HEIDELBERG, F.R. OF GERMANY)


                      INPUT DATA FOR CHANGES TO COMMON VARIABLES

LAST       0     1.00000E+00

IWT        0     5.00000E+00

IUSER     14     3.10000E+01

IUSER     15    -1.00000E+00

RUSER     14     1.00000E+00

RUSER     15     3.00000E-02

RUSER     16     5.00000E+02

END        0     0.00000E+00
NSTEND    51     2.40000E+02     1.90000E+02


                               FINAL VALUES OF CONTROL VARIABLES

DFMIN  = 3.00000E+00
SRMIN  = 1.00000E-02
ALPST  = 0.00000E+00 0.00000E+00
GMNMX  = 1.00000E+00 1.60000E+01
PLEVEL = 5.00000E-01 5.00000E-01 5.00000E-01 5.00000E-01
RSVMNX = 1.00000E+00 1.00000E+00 0.00000E+00 0.00000E+00
RUSER  = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 1.00000E+00 3.00000E-02 5.00000E+02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 IGRID  =          1
 IQUAD  =          1
 IUNIT  =         -1
 IWT    =          5
 LINEPG =         60
 MIOERR =          5
 MPKMOM =          0
 MQPITR =         35
 NEQ    =          0
 NERFIT =          0
 NG     =         16
 NINTT  =          1
 NLINF  =          0
 NORDER =         -1
 ICRIT  =          1          1
 IFORMT = (5E15.6)
 IFORMW = (5E15.6)
```

IFORMY =	(7F9.0)									
IPLFIT =	2	2								
IPLRES =	2	2								
IPRINT =	2	3								
IUSER =	0	0	0	0	0	0	0	0	0	
	0	0	0	31	-1	4	7	0	0	0
	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0
IUSROU =	3	3								
LSIGN =	0	0	0	0	0	0	0	0	0	
	0	0	0	0	0	0				
MOMNMX =	0	0								
NENDZ =	0	0								
NFLAT =	0	0	0	0	0	0	0	0		
NNSGN =	0	0								
NQPROG =	6	6								
NSGN =	0	0	0	0						
DOCHOS =	T									
DOMOM =	F									
DOUSIN =	T									
DOUSNQ =	T									
LAST =	T									
NEWPG1 =	T									
NONNEG =	F									
ONLY1 =	T									
PRWT =	T									
PRY =	T									
SIMULA =	F									
LUSER =	F	F	F	F	F	F	F	F	F	F
	F	F	F	F	F	F	F	F	F	F
	F	F	F	F	F	F	F	F	F	F

MAR 84 Page 12

T	Y	T	Y	T	Y	T	Y	T	Y
2.400E+02	-7.81000E+02	2.390E+02	-9.33000E+02	2.380E+02	-1.10700E+03	2.370E+02	-1.34500E+03	2.360E+02	-1.61700E+03
2.350E+02	-1.93100E+03	2.340E+02	-2.30000E+03	2.330E+02	-2.69100E+03	2.320E+02	-3.11400E+03	2.310E+02	-3.54800E+03
2.300E+02	-4.00300E+03	2.290E+02	-4.45800E+03	2.280E+02	-4.90300E+03	2.270E+02	-5.31500E+03	2.260E+02	-5.70600E+03
2.250E+02	-6.02100E+03	2.240E+02	-6.27000E+03	2.230E+02	-6.47600E+03	2.220E+02	-6.58400E+03	2.210E+02	-6.63900E+03
2.200E+02	-6.66100E+03	2.190E+02	-6.63900E+03	2.180E+02	-6.58500E+03	2.170E+02	-6.54100E+03	2.160E+02	-6.46500E+03
2.150E+02	-6.40000E+03	2.140E+02	-6.35700E+03	2.130E+02	-6.35700E+03	2.120E+02	-6.36800E+03	2.110E+02	-6.42200E+03
2.100E+02	-6.46500E+03	2.090E+02	-6.32400E+03	2.080E+02	-6.05300E+03	2.070E+02	-5.65200E+03	2.060E+02	-5.07700E+03
2.050E+02	-4.42600E+03	2.040E+02	-3.70900E+03	2.030E+02	-2.76200E+03	2.020E+02	-1.67700E+03	2.010E+02	-2.63000E+02
2.000E+02	1.21600E+03	1.990E+02	2.89400E+03	1.980E+02	4.50500E+03	1.970E+02	6.05000E+03	1.960E+02	7.36500E+03
1.950E+02	8.22000E+03	1.940E+02	8.91000E+03	1.930E+02	9.20600E+03	1.920E+02	9.23900E+03	1.910E+02	8.91300E+03
1.900E+02	8.41700E+03	0.000E+00	1.00000E+00						

PRECIS = 1.86D-16 SRANGE = 1.00E+35 RANGE = 1.00D+35

GRID POINT	MIN IN MATRIX A	AT T =	MAX IN MATRIX A	AT T =	SCALE FACTOR
1.0000E+00	-2.4876D+04	2.22D+02	5.5079D+04	1.92D+02	2.078D-06
2.0000E+00	-1.3387D+04	2.08D+02	1.7434D+04	1.92D+02	2.078D-06
3.0000E+00	-1.1109D+04	2.11D+02	1.6667D+04	0.00D+00	2.078D-06
4.0000E+00	-1.2593D+04	2.09D+02	1.6667D+04	0.00D+00	2.078D-06
5.0000E+00	-1.3227D+04	2.22D+02	2.4142D+04	1.93D+02	2.078D-06
6.0000E+00	-9.7762D+03	2.03D+02	1.6667D+04	0.00D+00	2.078D-06
7.0000E+00	-6.6914D+03	2.24D+02	1.6667D+04	0.00D+00	2.078D-06
8.0000E+00	-1.2254D+04	2.23D+02	1.6667D+04	0.00D+00	2.078D-06
9.0000E+00	-1.2473D+04	1.99D+02	1.6667D+04	0.00D+00	2.078D-06

1.0000E+01	-1.1208D+04	2.09D+02	1.6667D+04	0.00D+00	2.078D-06
1.1000E+01	-1.3714D+04	2.09D+02	2.5943D+04	1.96D+02	2.078D-06
1.2000E+01	-1.4514D+04	2.22D+02	1.9732D+04	1.95D+02	2.078D-06
1.3000E+01	-9.9252D+03	2.12D+02	1.6667D+04	0.00D+00	2.078D-06
1.4000E+01	-1.8628D+04	2.03D+02	1.6667D+04	0.00D+00	2.078D-06
1.5000E+01	-1.4012D+04	2.10D+02	2.8231D+04	1.92D+02	2.078D-06
1.6000E+01	-1.1083D+04	2.11D+02	1.6667D+04	0.00D+00	2.078D-06

SCALE FACTOR FOR ALPHA = 7.700E+06

0 UNREGULARIZED VARIABLES

SINGULAR VALUES

4.036E-02	1.461E-02	6.268E-03	3.163E-03	1.902E-03	1.817E-03	1.383E-03	5.122E-04	4.872E-04	3.099E-04
2.796E-04	1.190E-04	8.184E-05	6.539E-05	2.937E-05	2.580E-05				

TEST DATA SET 2 - FOR CD PACKAGE

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 7.52E-18	1.86E-16	5.20198E+04	5.20198E+04	3.801E+01	16.000	0.000	1.000

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.16	0.48	0.36	1.000
STANDARD ERROR	9.8E-03	9.6E-03	1.7E-02	

(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.0347 PUNCOR = 0.1222 0.3862 0.0344 0.0001 0.0055

MAR 84 Page 14

TEST DATA SET 2 - FOR CD PACKAGE

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 8.36E-15	2.07E-13	5.20198E+04	5.20198E+04	3.801E+01	16.000	0.000	1.000

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.16	0.48	0.36	1.000
STANDARD ERROR	9.8E-03	9.6E-03	1.7E-02	

(FOR ALPHA/S(1) = 2.07E-13) PRUNS = 0.0347 PUNCOR = 0.1222 0.3862 0.0344 0.0001 0.0055

TEST DATA SET 2 - FOR CD PACKAGE

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
* 9.29E-12	2.30E-10	5.20198E+04	5.20198E+04	3.801E+01	16.000	0.000	1.000

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.16	0.48	0.36	1.000
STANDARD ERROR	9.8E-03	9.6E-03	1.7E-02	

(FOR ALPHA/S(1) = 2.30E-10) PRUNS = 0.0347 PUNCOR = 0.1222 0.3862 0.0344 0.0001 0.0055

TEST DATA SET 2 - FOR CD PACKAGE

PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.03E-08	2.56E-07	5.20198E+04	5.20198E+04	3.801E+01	16.000	0.000	1.000

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.16	0.48	0.36	1.000
STANDARD ERROR	9.8E-03	9.6E-03	1.7E-02	

(FOR ALPHA/S(1) = 2.56E-07) PRUNS = 0.0347 PUNCOR = 0.1222 0.3862 0.0344 0.0001 0.0055

TEST DATA SET 2 - FOR CD PACKAGE

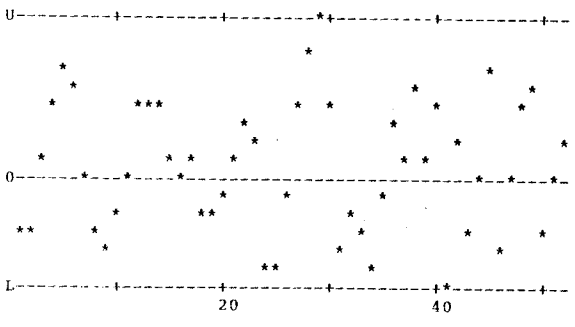
PRELIMINARY UNWEIGHTED ANALYSIS

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
1.15E-05	2.84E-04	6.04280E+04	5.24436E+04	3.798E+01	15.640	0.000	0.746

	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.16	0.49	0.36	1.000
STANDARD ERROR	8.9E-03	8.7E-03	1.5E-02	

(FOR ALPHA/S(1) = 2.84E-04) PRUNS = 0.0347 PUNCOR = 0.0808 0.4531 0.0245 0.0001 0.0045

WEIGHTED RESIDUALS (ALPHA/S(1)= 7.75E-04) MAX=U= 8.2E+01 MIN=L=-6.1E+01 (PRUNS= 0.0089) PUNCOR= 0.0114 0.7774 0.0150 0.0002 0.0025



MAR 84 Page 17

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

ORDINATE	ABSCISSA	
-7.503E+02	2.40E+02	
-8.969E+02	2.39E+02	
-1.113E+03	2.38E+02	
-1.378E+03	2.37E+02	
-1.670E+03	2.36E+02	
-1.972E+03	2.35E+02	
-2.292E+03	2.34E+02	
-2.658E+03	2.33E+02	
-3.074E+03	2.32E+02	
-3.520E+03	2.31E+02	
-4.003E+03	2.30E+02	
-4.493E+03	2.29E+02	XO
-4.937E+03	2.28E+02	XO
-5.350E+03	2.27E+02	XO
-5.713E+03	2.26E+02	*
-6.022E+03	2.25E+02	*
-6.275E+03	2.24E+02	*
-6.451E+03	2.23E+02	*
-6.560E+03	2.22E+02	*
-6.628E+03	2.21E+02	*
-6.662E+03	2.20E+02	*
-6.659E+03	2.19E+02	*
-6.596E+03	2.18E+02	*
-6.494E+03	2.17E+02	OX
-6.417E+03	2.16E+02	*
-6.388E+03	2.15E+02	*
-6.391E+03	2.14E+02	XO
-6.420E+03	2.13E+02	XO
-6.450E+03	2.12E+02	XO
-6.458E+03	2.11E+02	*
-6.419E+03	2.10E+02	*
-6.298E+03	2.09E+02	*
-6.019E+03	2.08E+02	*
-5.603E+03	2.07E+02	OX

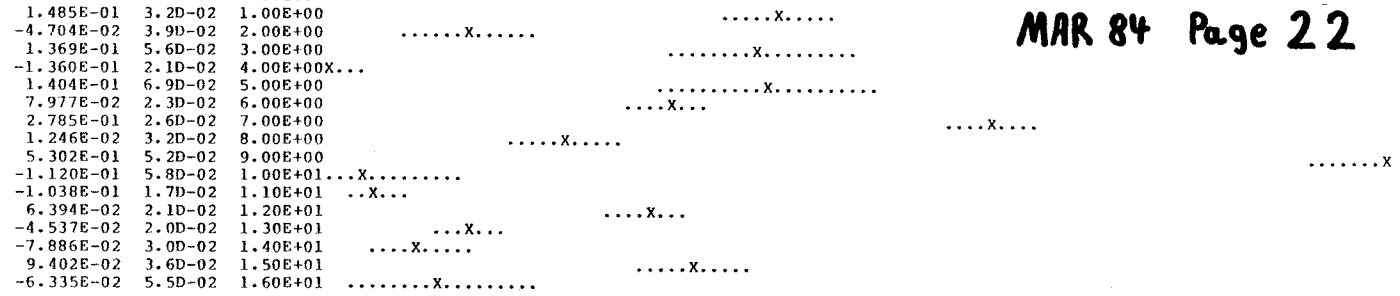
MAR 84 Page 18

```
-5.063E+03  2.06E+02           *
-4.451E+03  2.05E+02                *
-3.715E+03  2.04E+02                     *
-2.806E+03  2.03E+02                           *
-1.685E+03  2.02E+02                                   *
-2.983E+02  2.01E+02                                            *
 1.277E+03  2.00E+02                                                       *
 2.883E+03  1.99E+02                                                                  *
 4.535E+03  1.98E+02                                                                             *
 6.057E+03  1.97E+02                                                                                        *
 7.310E+03  1.96E+02                                                                                                XO
 8.267E+03  1.95E+02                                                                                                        *
 8.918E+03  1.94E+02                                                                                                            *
 9.169E+03  1.93E+02                                                                                                              *
 9.198E+03  1.92E+02                                                                                                              *
 8.950E+03  1.91E+02                                                                                                           OX
 8.421E+03  1.90E+02                                                                                                         *
 9.993E-01  0.00E+00                                              *


RMS RESIDUAL FOR PTS. 1 TO 31 =   3.44E+01
RMS RESIDUAL FOR REMAINING PTS. = 3.38E+01


ERRFIT = 0.00E+00
                          SQUARE ROOTS OF LEAST SQUARES WEIGHTS
   2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02
   2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02
   2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02
   2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02
   2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02    2.9277E-02
   2.9277E-02    3.3333E+01


  GRID POINT     MIN IN MATRIX A    AT T =     MAX IN MATRIX A    AT T =     SCALE FACTOR
  1.0000E+00         -7.2830D+02  2.22D+02          1.6125D+03  1.92D+02        7.334D-05
  2.0000E+00         -3.9192D+02  2.08D+02          5.1041D+02  1.92D+02        7.334D-05
  3.0000E+00         -3.2523D+02  2.11D+02          1.8973D+02  1.94D+02        7.334D-05
  4.0000E+00         -3.6870D+02  2.09D+02          4.3332D+02  1.90D+02        7.334D-05
  5.0000E+00         -3.8724D+02  2.22D+02          7.0681D+02  1.93D+02        7.334D-05
  6.0000E+00         -2.8622D+02  2.03D+02          1.1921D+02  1.90D+02        7.334D-05
  7.0000E+00         -1.9591D+02  2.24D+02          3.5119D+02  1.97D+02        7.334D-05
  8.0000E+00         -3.5876D+02  2.23D+02          3.7945D+02  1.96D+02        7.334D-05
  9.0000E+00         -3.6517D+02  1.99D+02          3.3333D+01  0.00D+00        7.334D-05
  1.0000E+01         -3.2813D+02  2.09D+02          3.6276D+02  1.90D+02        7.334D-05
  1.1000E+01         -4.0152D+02  2.09D+02          7.5953D+02  1.96D+02        7.334D-05
  1.2000E+01         -4.2493D+02  2.22D+02          5.7768D+02  1.95D+02        7.334D-05
  1.3000E+01         -2.9058D+02  2.12D+02          4.2974D+02  1.98D+02        7.334D-05
  1.4000E+01         -5.4537D+02  2.03D+02          1.4844D+02  1.90D+02        7.334D-05
  1.5000E+01         -4.1023D+02  2.10D+02          8.2652D+02  1.92D+02        7.334D-05
  1.6000E+01         -3.2449D+02  2.11D+02          1.9207D+02  1.95D+02        7.334D-05
SCALE FACTOR FOR ALPHA =  2.182E+05

  0 UNREGULARIZED VARIABLES

SINGULAR VALUES
    4.101E-02     1.469E-02     5.934E-03     3.173E-03     1.920E-03     1.452E-03     5.741E-04     5.167E-04     4.198E-04     3.111E-04
    1.827E-04     9.533E-05     8.205E-05     5.424E-05     2.853E-05     2.660E-05
```

TEST DATA SET 2 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
3.18E-05	7.75E-04	7.05746E+01	4.91824E+01	1.142E+00	14.319	0.035	0.968

ORDINATE	ERROR	ABSCISSA
1.485E-01	3.2D-02	1.00E+00
-4.704E-02	3.9D-02	2.00E+00
1.369E-01	5.6D-02	3.00E+00
-1.360E-01	2.1D-02	4.00E+00
1.404E-01	6.9D-02	5.00E+00
7.977E-02	2.3D-02	6.00E+00
2.785E-01	2.6D-02	7.00E+00
1.246E-02	3.2D-02	8.00E+00
5.302E-01	5.2D-02	9.00E+00
-1.120E-01	5.8D-02	1.00E+01
-1.038E-01	1.7D-02	1.10E+01
6.394E-02	2.1D-02	1.20E+01
-4.537E-02	2.0D-02	1.30E+01
-7.886E-02	3.0D-02	1.40E+01
9.402E-02	3.6D-02	1.50E+01
-6.335E-02	5.5D-02	1.60E+01



	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.18	0.47	0.35	0.898
STANDARD ERROR	7.2E-03	2.1E-02	1.6E-02	

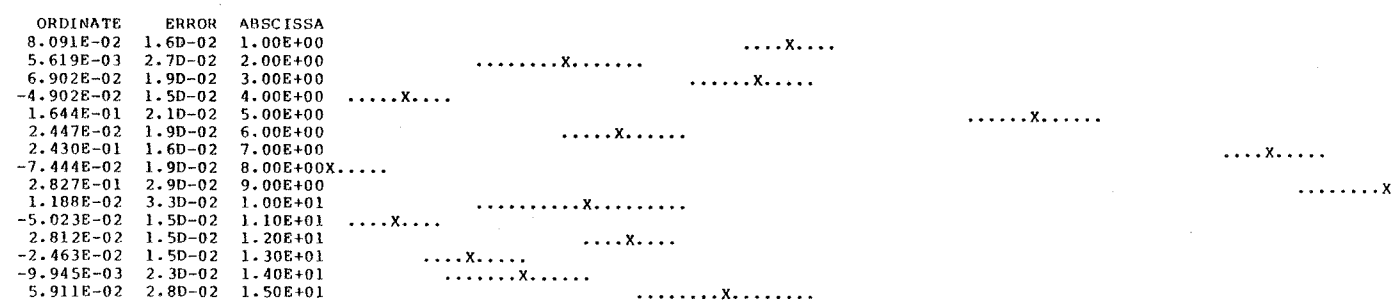
(FOR ALPHA/S(1) = 7.75E-04) PRUNS = 0.1105 PUNCOR = 0.1015 0.3476 0.1311 0.0238 0.0341

MAR 84 Page 22

TEST DATA SET 2 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
8.65E-05	2.11E-03	1.43634E+02	8.74182E+01	1.481E+00	12.136	0.989	1.000

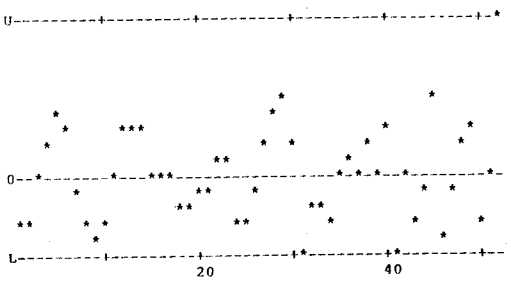
ORDINATE	ERROR	ABSCISSA
8.091E-02	1.6D-02	1.00E+00
5.619E-03	2.7D-02	2.00E+00
6.902E-02	1.9D-02	3.00E+00
-4.902E-02	1.5D-02	4.00E+00
1.644E-01	2.1D-02	5.00E+00
2.447E-02	1.9D-02	6.00E+00
2.430E-01	1.6D-02	7.00E+00
-7.444E-02	1.9D-02	8.00E+00
2.827E-01	2.9D-02	9.00E+00
1.188E-02	3.3D-02	1.00E+01
-5.023E-02	1.5D-02	1.10E+01
2.812E-02	1.5D-02	1.20E+01
-2.463E-02	1.5D-02	1.30E+01
-9.945E-03	2.3D-02	1.40E+01
5.911E-02	2.8D-02	1.50E+01
3.650E-02	1.8D-02	1.60E+01



	HELIX	BETA-SHEET	REMAINDER	SCALE FACTOR
FRACTION	0.21	0.44	0.36	0.798
STANDARD ERROR	5.4E-03	1.8E-02	1.5E-02	

(FOR ALPHA/S(1) = 2.11E-03) PRUNS = 0.0089 PUNCOR = 0.3983 0.6474 0.8429 0.3719 0.2669

WEIGHTED RESIDUALS (ALPHA/S(1)= 7.75E-04) MAX=U= 3.4E+00 MIN=L=-1.5E+00 (PRUNS= 0.1105) PUNCOR= 0.1015 0.3476 0.1311 0.0238 0.0341



MAR 84 Page 25

PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

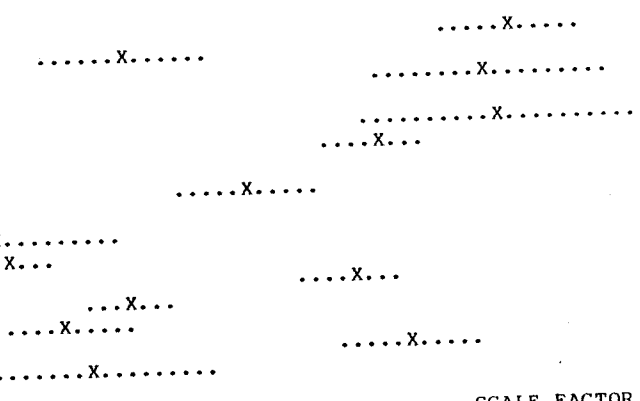
ORDINATE	ABSCISSA
-7.493E+02	2.40E+02
-8.998E+02	2.39E+02
-1.114E+03	2.38E+02
-1.375E+03	2.37E+02
-1.663E+03	2.36E+02
-1.967E+03	2.35E+02
-2.292E+03	2.34E+02
-2.659E+03	2.33E+02
-3.075E+03	2.32E+02
-3.522E+03	2.31E+02
-4.002E+03	2.30E+02
-4.491E+03	2.29E+02
-4.937E+03	2.28E+02
-5.348E+03	2.27E+02
-5.710E+03	2.26E+02
-6.019E+03	2.25E+02
-6.273E+03	2.24E+02
-6.453E+03	2.23E+02
-6.564E+03	2.22E+02
-6.628E+03	2.21E+02
-6.658E+03	2.20E+02
-6.654E+03	2.19E+02
-6.598E+03	2.18E+02
-6.506E+03	2.17E+02
-6.431E+03	2.16E+02
-6.393E+03	2.15E+02
-6.385E+03	2.14E+02
-6.402E+03	2.13E+02
-6.431E+03	2.12E+02
-6.447E+03	2.11E+02
-6.416E+03	2.10E+02
-6.302E+03	2.09E+02
-6.035E+03	2.08E+02
-5.621E+03	2.07E+02
-5.075E+03	2.06E+02
-4.444E+03	2.05E+02
-3.708E+03	2.04E+02
-2.793E+03	2.03E+02
-1.678E+03	2.02E+02
-3.055E+02	2.01E+02
1.269E+03	2.00E+02
2.832E+03	1.99E+02
4.532E+03	1.98E+02
6.054E+03	1.97E+02
7.309E+03	1.96E+02
8.264E+03	1.95E+02
8.916E+03	1.94E+02
9.178E+03	1.93E+02
9.203E+03	1.92E+02
8.949E+03	1.91E+02
8.418E+03	1.90E+02
8.981E-01	0.00E+00

CONTIN VERSION 2DP (MAR 1984) (CD-1 PACKAGE) ++++++++++++++++++++++++++++++++ CHOSEN SOLUTION ++++++++++++++++++++++++++++++++

TEST DATA SET 2 - FOR CD PACKAGE

ALPHA	ALPHA/S(1)	OBJ. FCTN.	VARIANCE	STD. DEV.	DEG FREEDOM	PROB1 TO REJECT	PROB2 TO REJECT
3.18E-05	7.75E-04	7.05746E+01	4.91824E+01	1.142E+00	14.319	0.035	0.968

ORDINATE	ERROR	ABSCISSA
1.485E-01	3.2D-02	1.00E+00
-4.704E-02	3.9D-02	2.00E+00
1.369E-01	5.6D-02	3.00E+00
-1.360E-01	2.1D-02	4.00E+00
1.404E-01	6.9D-02	5.00E+00
7.977E-02	2.3D-02	6.00E+00
2.785E-01	2.6D-02	7.00E+00
1.246E-02	3.2D-02	8.00E+00
5.302E-01	5.2D-02	9.00E+00
-1.120E-01	5.8D-02	1.00E+01
-1.038E-01	1.7D-02	1.10E+01
6.394E-02	2.1D-02	1.20E+01
-4.537E-02	2.0D-02	1.30E+01
-7.886E-02	3.0D-02	1.40E+01
9.402E-02	3.6D-02	1.50E+01
-6.335E-02	5.5D-02	1.60E+01



	HELIX	BETA-SHEET	REMAINDER
FRACTION	0.18	0.47	0.35
STANDARD ERROR	7.2E-03	2.1E-02	1.6E-02

SCALE FACTOR 0.898

MAR 84 Page 27