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.

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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

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

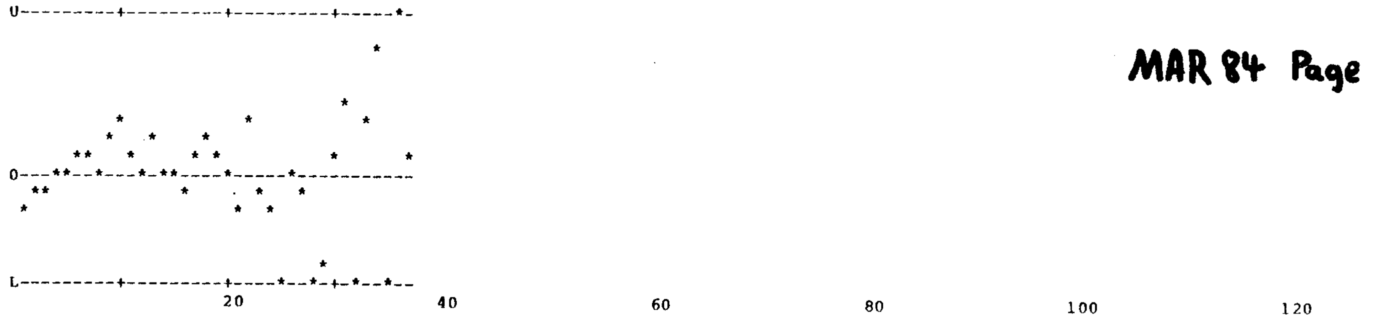
(FOR ALPHA/S(1) = 2.52E-12) PRUNS = 0.1597 PUNCOR = 0.5188 0.9485 0.0103 0.6535 0.6671

MAR 84 Page 12

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

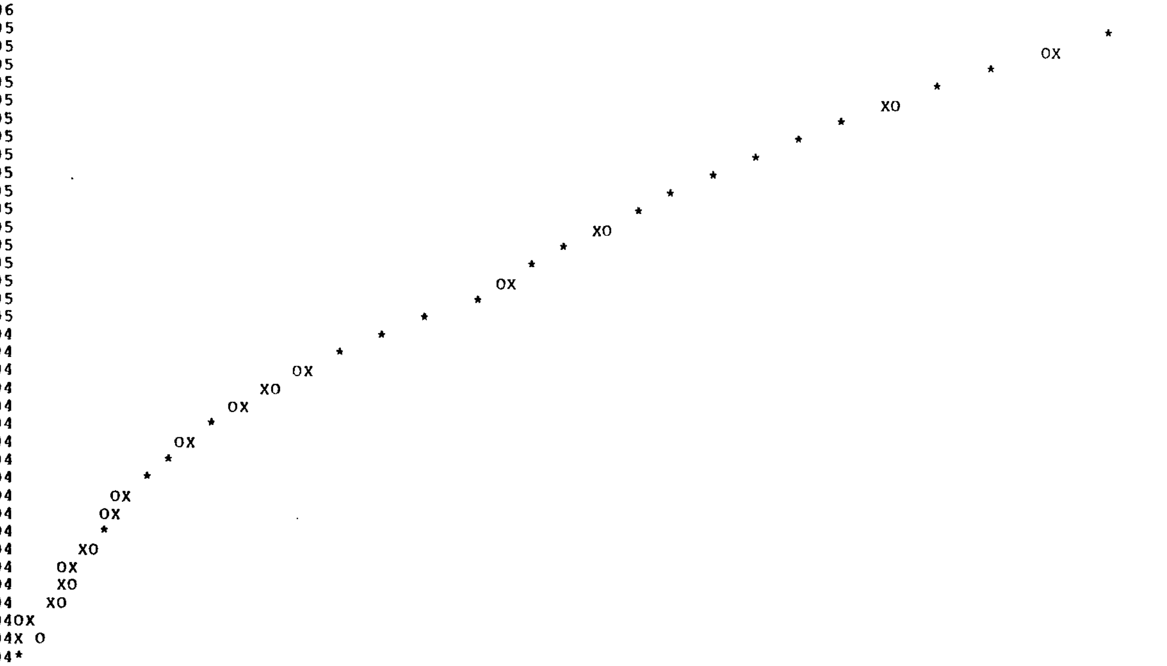
WEIGHTED RESIDUALS (ALPHA/S(1)= 2.52E-12) MAX=U= 8.1E-03 MIN=L=-5.6E-03 (PRUNS= 0.1597) PUNCOR= 0.5188 0.9485 0.0103 0.6535 0.6671

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

.....X.....

....X

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

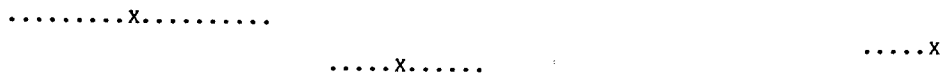
(FOR ALPHA/S(1) = 2.03E-12) PRUNS = 0.1671 PUNCOR = 0.5745 0.8722 0.0873 0.1388 0.8420

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

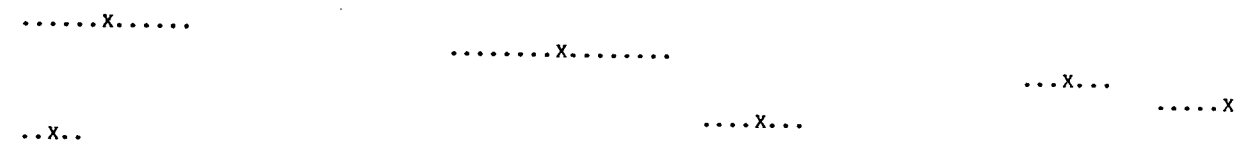
J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
-1	1.9502 X (10** -11)	5.0E+00			
0	3.4143 X (10** -6)	1.3E+00	1.7507E+05	6.3E+00	0
1	6.2188 X (10** -1)	3.5E-01	1.8214E+05	1.6E+00	1
2	1.1758 X (10** 5)	2.9E+00	1.8907E+05	3.2E+00	2
3	2.3023 X (10** 10)	8.3E+00	1.9581E+05	1.1E+01	3

(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

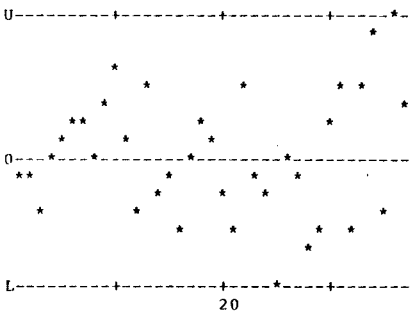
PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(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

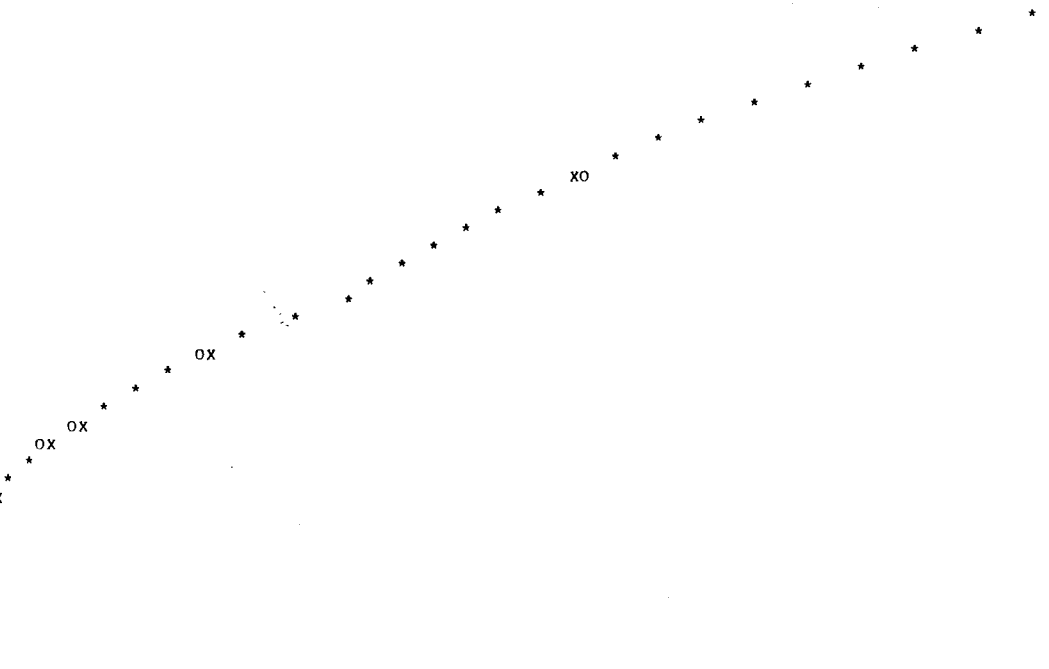
(FOR ALPHA/S(1) = 3.16E-12) PRUNS = 0.0479 PUNCOR = 0.3958 0.6727 0.0625 0.1177 0.9101

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

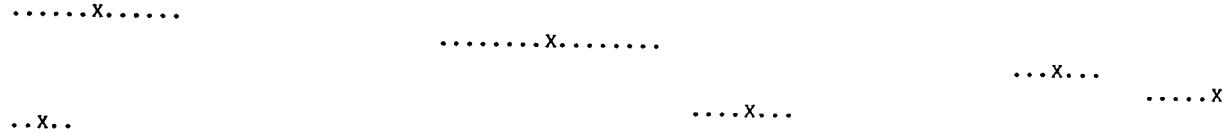


CONTIN VERSION 2DP (MAR 1984) (PCS-1 PACKAGE) ++++++++++++++++++++++++++++++++ CHOSEN SOLUTION ++++++++++++++++++++++++++++++++

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

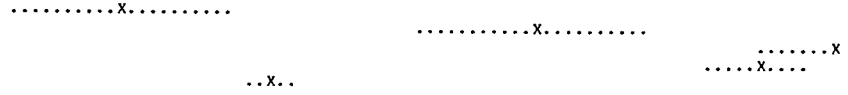
(FOR ALPHA/S(1) = 1.00E-10) PRUNS = 0.0105 PUNCOR = 0.0210 0.0450 0.0005 0.2231 0.9776

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

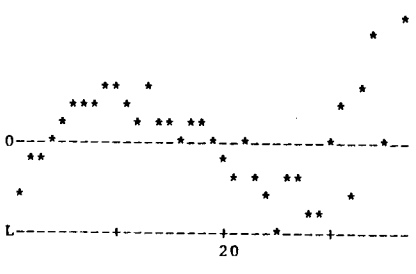
PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(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

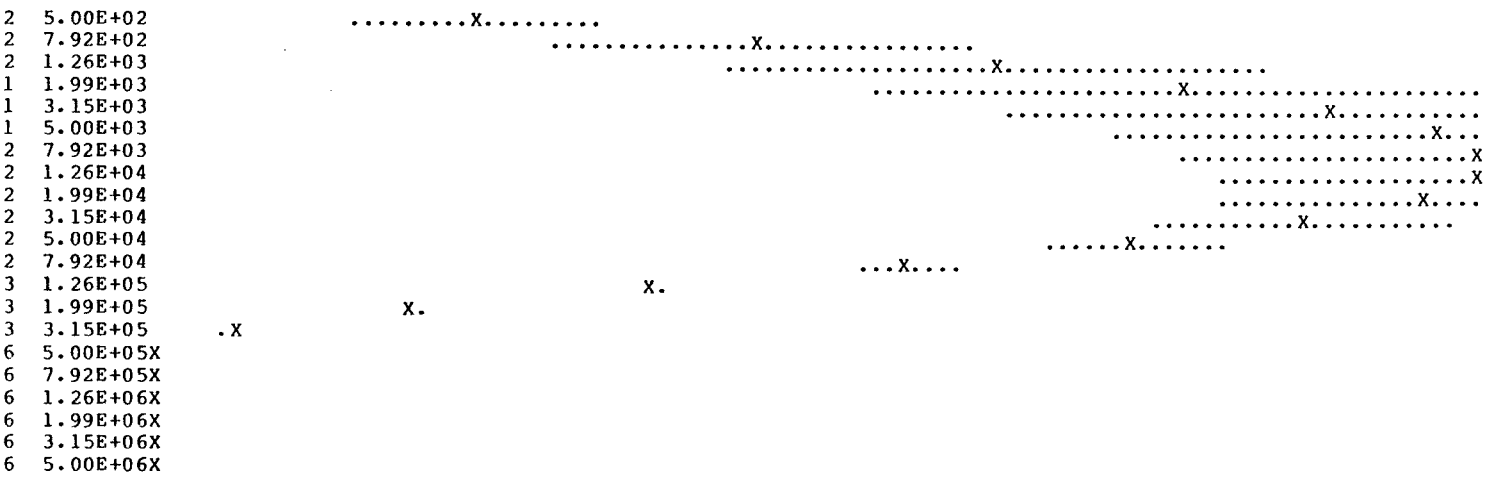
ALPHA = 5.83E-05 ALPHA/S(1) = 7.35E-06

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



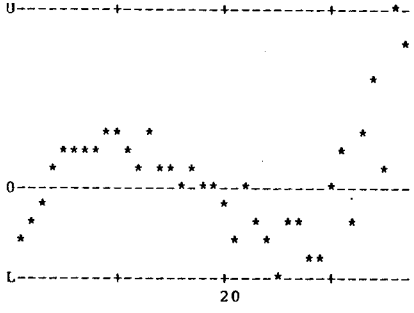
PEAK 1 GOES FROM 5.000E+02 TO 5.000E+06

(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

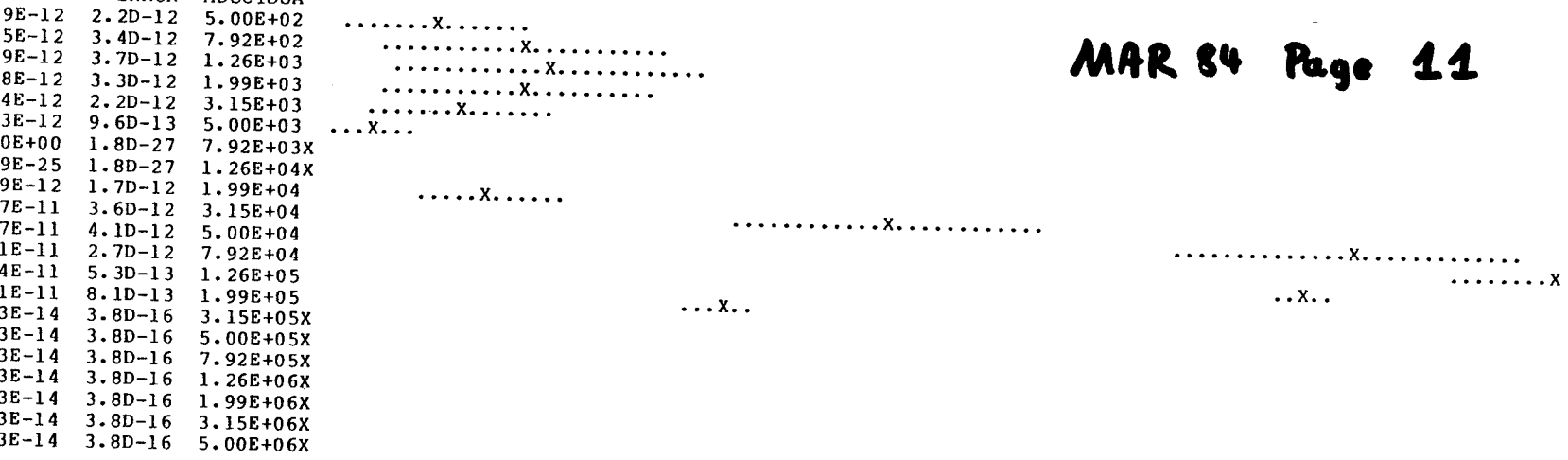
MAR 84 Page 10

	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

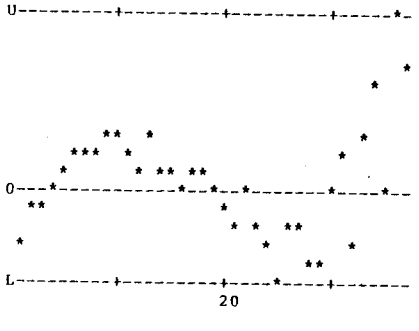
MOMENTS OF ENTIRE SOLUTION

(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



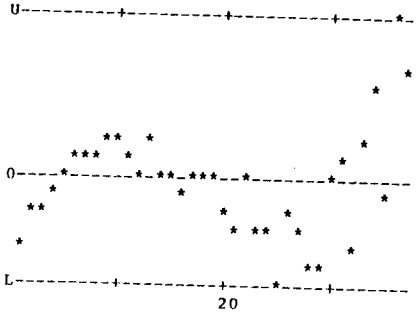
MAR 84 Page 12

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)

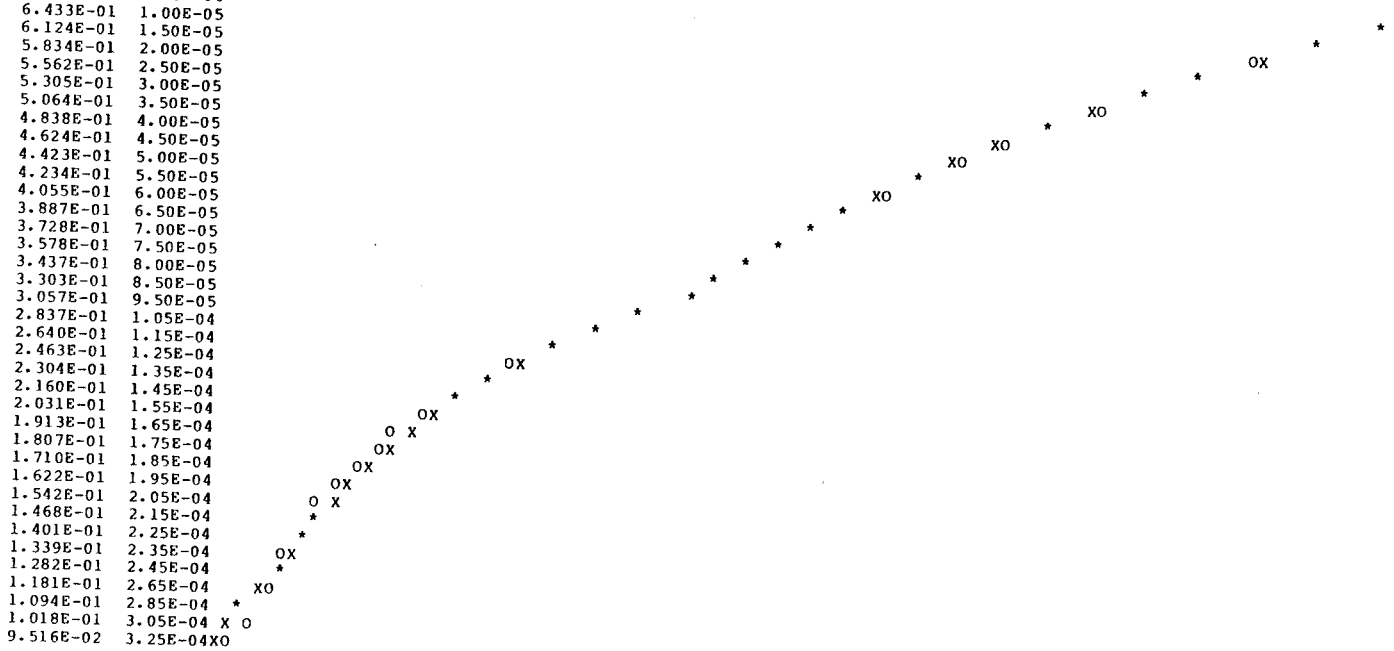
WEIGHTED RESIDUALS (ALPHA/S(1)= 1.00E-06) MAX=U= 1.4E-02 MIN=L=-8.3E-03 (PRUNS= 0.0105) PUNCOR= 0.0031 0.0116 0.0002 0.1496 0.8836 CHOSEN SOLUTION



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

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

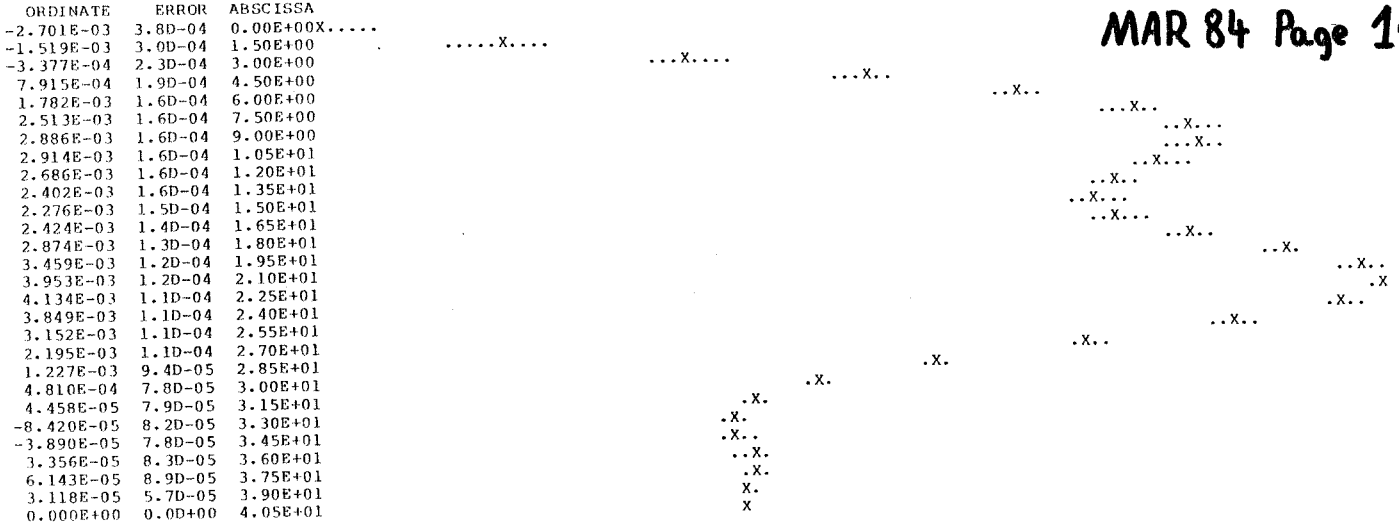
TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

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

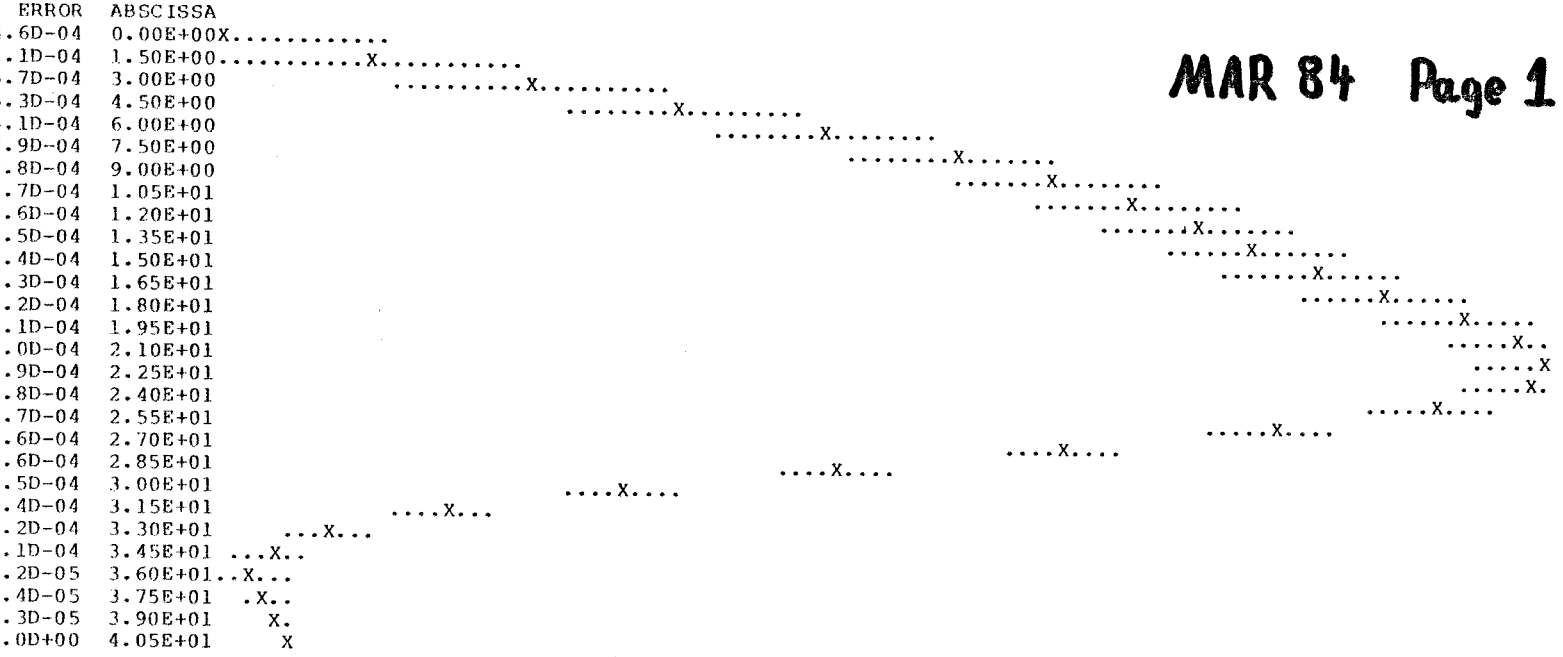
TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

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

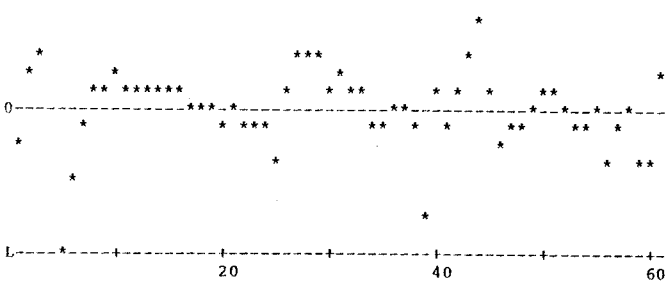
MOMENTS OF ENTIRE SOLUTION

(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

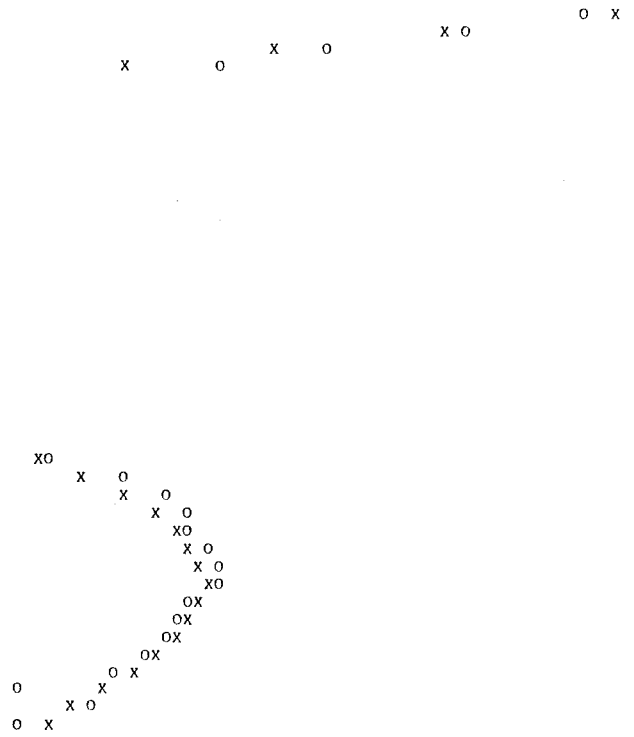
WEIGHTED RESIDUALS (ALPHA/S(1)= 5.75E-03) MAX=U= 2.5E-01 MIN=L=-3.1E-01 (PRUNS= 0.0000) PUNCOR= 0.0818 0.6547 0.2590 0.7581 0.2042



MAR 84 Page 16

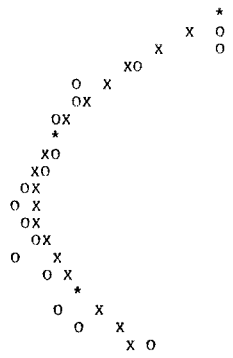
PLOT OF DATA (O) AND FIT TO DATA (X). ORDINATES LISTED ARE FIT VALUES.

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

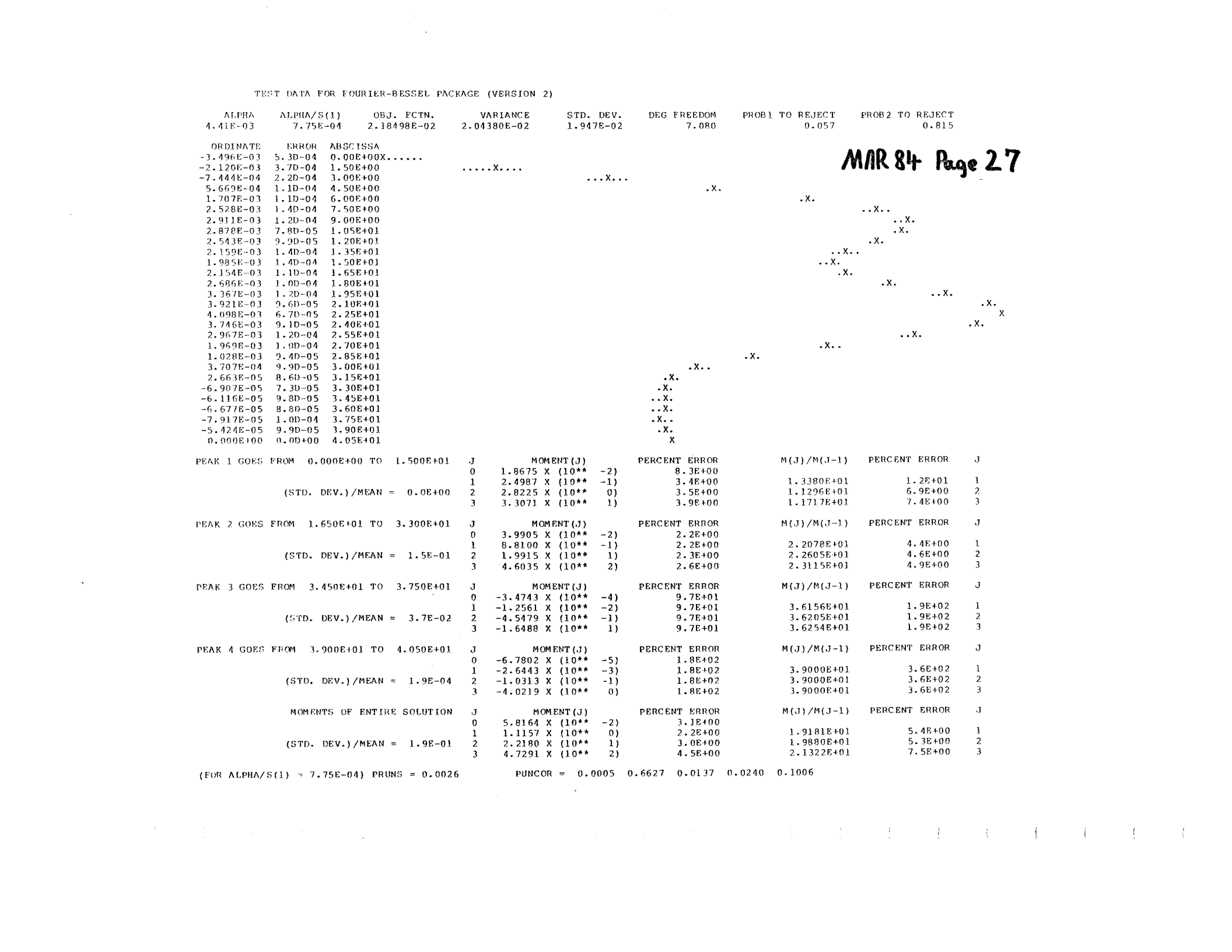
(FOR ALPHA/S(1) = 1.86E-16) PRUNS = 0.0363 PUNCOR = 0.0033 0.2130 0.0007 0.0218 0.2800

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

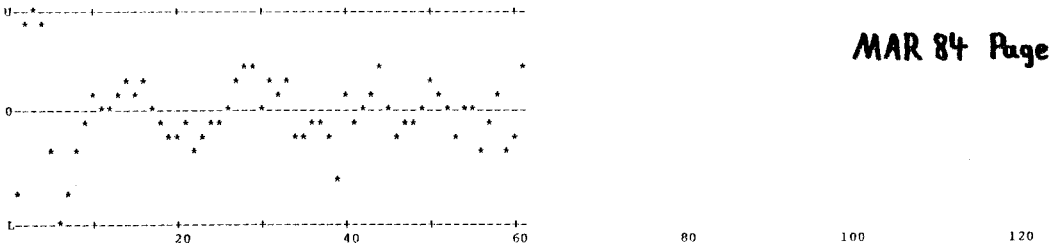


	J	MOMENT(J)	PERCENT ERROR	M(J)/M(J-1)	PERCENT ERROR	J
PEAK 1 GOES FROM 0.000E+00 TO 1.500E+01	0	1.8675 X (10** -2)	8.3E+00			
	1	2.4987 X (10** -1)	3.4E+00	1.3380E+01	1.2E+01	1
(STD. DEV.)/MEAN = 0.0E+00	2	2.8225 X (10** 0)	3.5E+00	1.1296E+01	6.9E+00	2
	3	3.3071 X (10** 1)	3.9E+00	1.1717E+01	7.4E+00	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

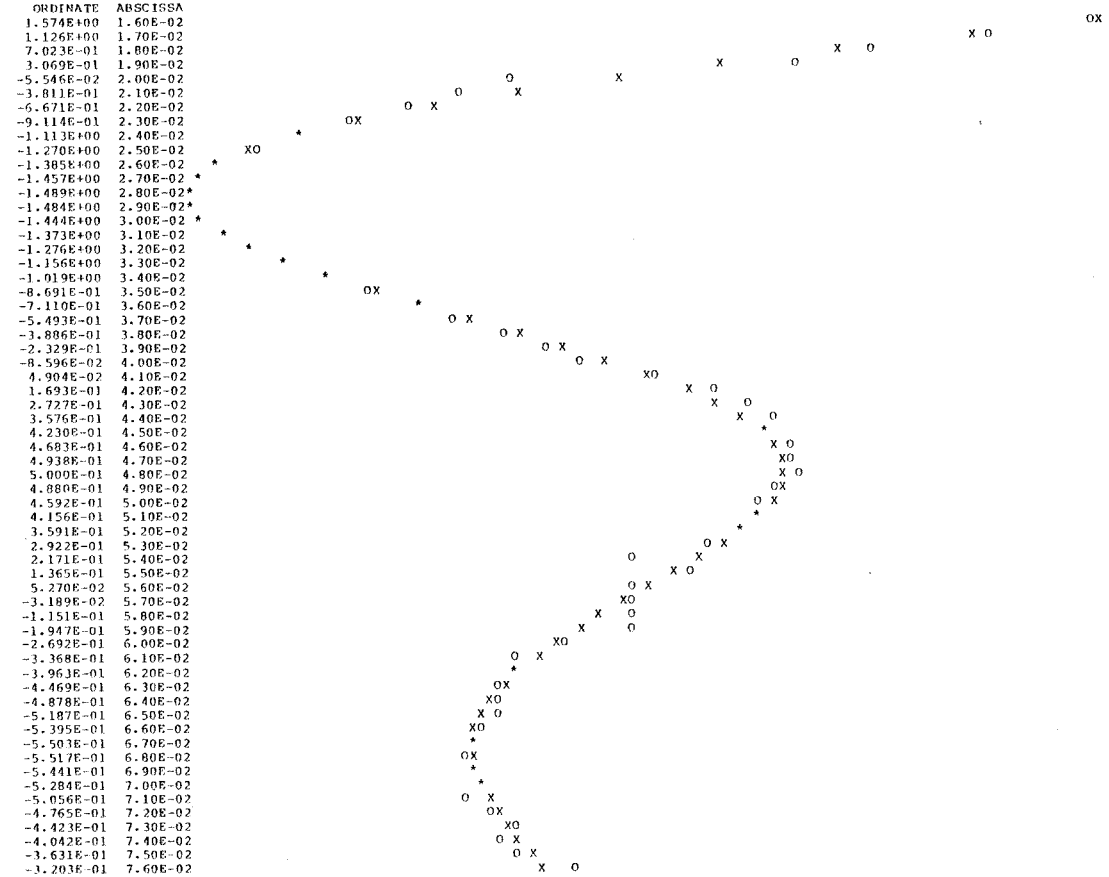
WEIGHTED RESIDUALS (ALPHA/S(1)= 7.75E-04) MAX=U= 4.9E-02 MIN=L=-5.3E-02 (PRUNS= 0.0026) PUNCOR= 0.0005 0.6627 0.0137 0.0240 0.1006



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

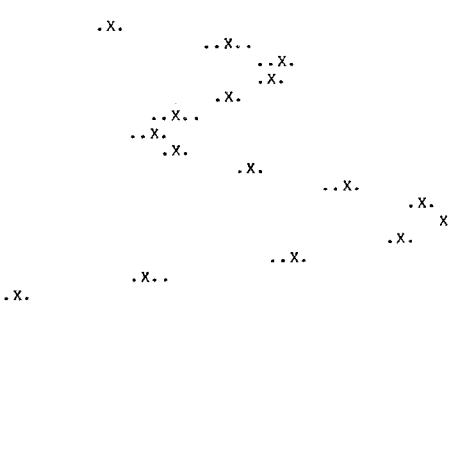


TEST DATA FOR FOURIER-BESSEL PACKAGE (VERSION 2)

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

```
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
```

MAR 84 Page 1

```
                                  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
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         0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
         0.00000E+00 0.00000E+00 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

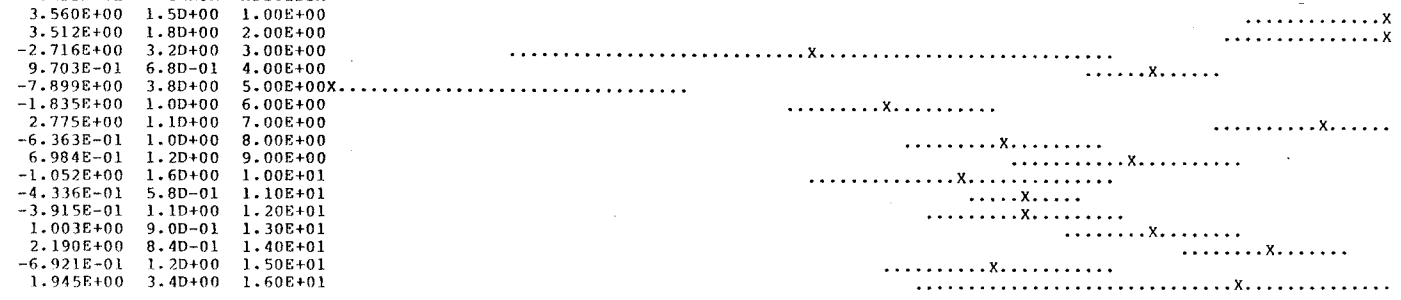
SINGULAR VALUES

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	

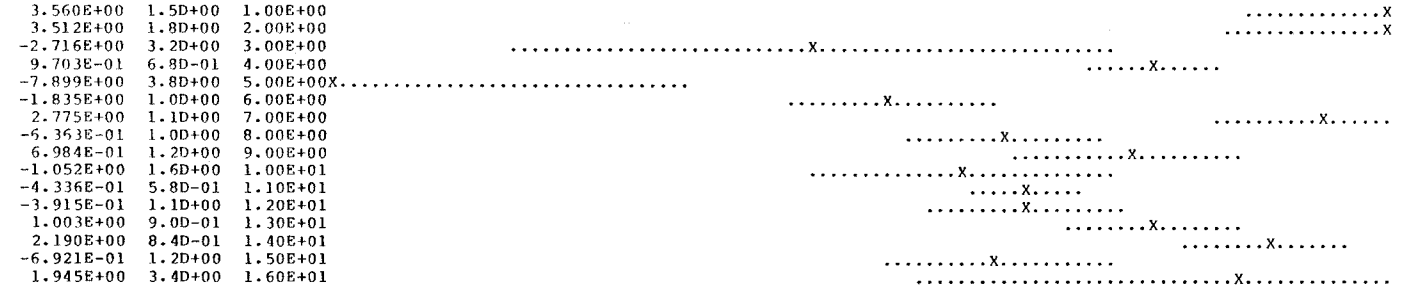
MAR 84 Page 3

(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

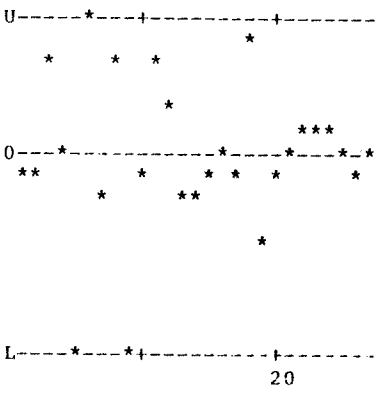
ORDINATE	ERROR	ABSCISSA
3.560E+00	1.5D+00	1.00E+00
3.512E+00	1.8D+00	2.00E+00
-2.716E+00	3.2D+00	3.00E+00
9.703E-01	6.8D-01	4.00E+00
-7.899E+00	3.8D+00	5.00E+00
-1.835E+00	1.0D+00	6.00E+00
2.775E+00	1.1D+00	7.00E+00
-6.363E-01	1.0D+00	8.00E+00
6.984E-01	1.2D+00	9.00E+00
-1.052E+00	1.6D+00	1.00E+01
-4.336E-01	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.

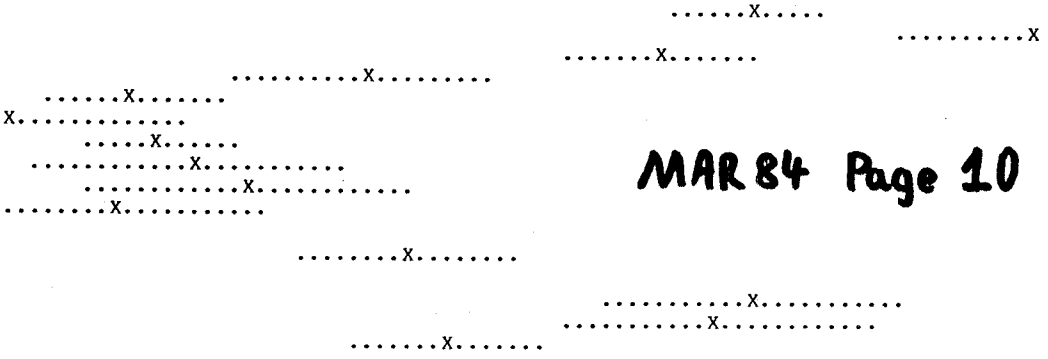
ORDINATE	ABSCISSA
4.704E+04	1.90E+02
4.447E+04	1.92E+02
3.508E+04	1.94E+02
2.022E+04	1.96E+02
4.460E+03	1.98E+02
-7.884E+03	2.00E+02
-1.948E+04	2.02E+02
-2.732E+04	2.04E+02
-2.869E+04	2.06E+02
-2.787E+04	2.08E+02
-2.592E+04	2.10E+02
-2.382E+04	2.12E+02
-2.266E+04	2.14E+02
-2.253E+04	2.16E+02
-2.302E+04	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

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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)
```

MAR 84 Page 11

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

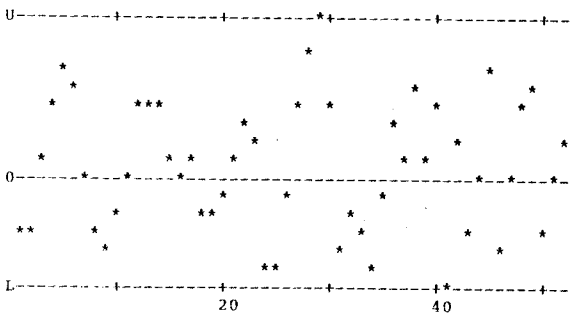
PRELIMINARY UNWEIGHTED ANALYSIS

	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

```
-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

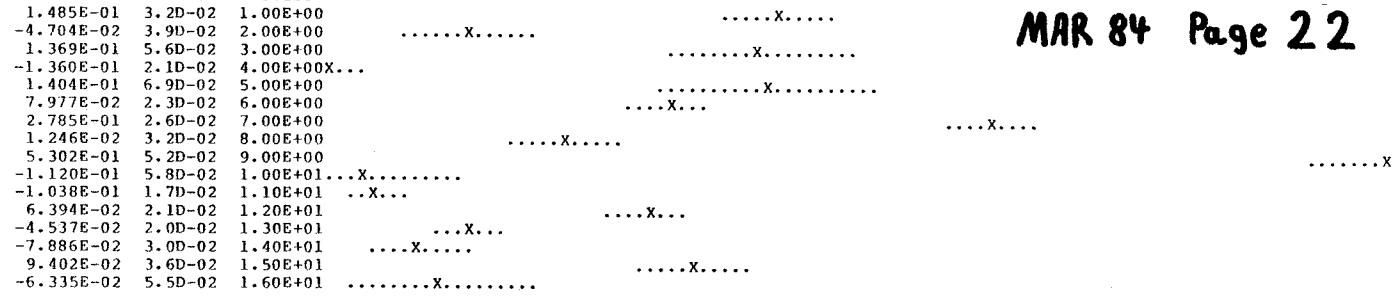
 0 UNREGULARIZED VARIABLES

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	

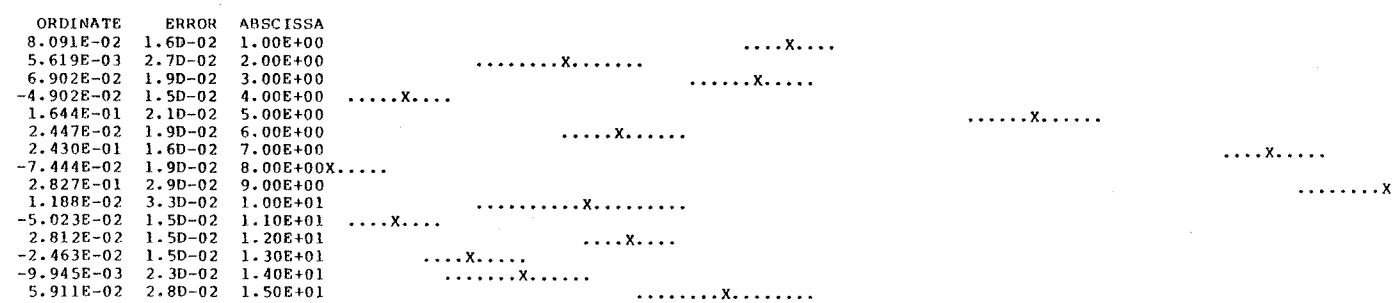
(FOR ALPHA/S(1) = 7.75E-04) PRUNS = 0.1105 PUNCOR = 0.1015 0.3476 0.1311 0.0238 0.0341

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

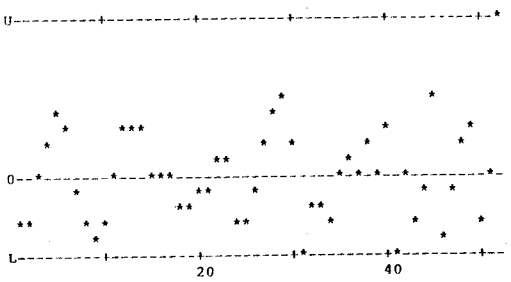
ORDINATE	ERROR	ABSCISSA
8.091E-02	1.6D-02	1.00E+00
5.619E-03	2.7D-02	2.00E+00
6.902E-02	1.9D-02	3.00E+00
-4.902E-02	1.5D-02	4.00E+00
1.644E-01	2.1D-02	5.00E+00
2.447E-02	1.9D-02	6.00E+00
2.430E-01	1.6D-02	7.00E+00
-7.444E-02	1.9D-02	8.00E+00
2.827E-01	2.9D-02	9.00E+00
1.188E-02	3.3D-02	1.00E+01
-5.023E-02	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.

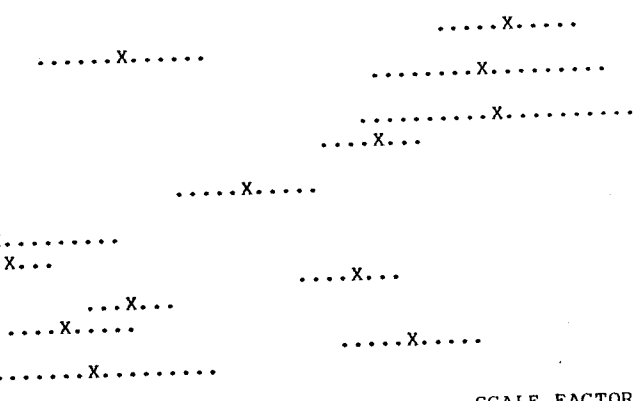
ORDINATE	ABSCISSA
-7.493E+02	2.40E+02
-8.998E+02	2.39E+02
-1.114E+03	2.38E+02
-1.375E+03	2.37E+02
-1.663E+03	2.36E+02
-1.967E+03	2.35E+02
-2.292E+03	2.34E+02
-2.659E+03	2.33E+02
-3.075E+03	2.32E+02
-3.522E+03	2.31E+02
-4.002E+03	2.30E+02
-4.491E+03	2.29E+02
-4.937E+03	2.28E+02
-5.348E+03	2.27E+02
-5.710E+03	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