

# PEST RUN RECORD: CASE mfit

PEST Version: 16.1

PEST run mode:-

Parameter estimation mode

Case dimensions:-

|                                 |   |     |
|---------------------------------|---|-----|
| Number of parameters            | : | 12  |
| Number of adjustable parameters | : | 12  |
| Number of parameter groups      | : | 1   |
| Number of observations          | : | 500 |
| Number of prior estimates       | : | 0   |

Model command line(s):-

MDP\_2RNE

Jacobian command line:-

MDP\_2RNE /d  
Jacobian read from file Deriv.txt  
This is an ASCII file.

Model interface files:-

Templates:  
MFIT.tpl  
for model input files:  
Input.txt  
  
(Parameter values written using single precision protocol.)  
(Decimal point always included.)  
  
Instruction files:  
MFIT.ins  
for reading model output files:  
Output.txt

PEST-to-model message file:-

na

Singular value decomposition:-

|  |   |              |
|--|---|--------------|
| Perform SVD on $XtQX$ or $Q^{(1/2)}X$    | : | $Q^{(1/2)}X$ |
| Max. number of singular values to employ | : | 12           |
| Ratio of lowest/highest singular value   | : | 5.000000E-07 |
| Record eigenvectors in SVD file          | : | yes          |

Derivatives calculation:-

| Param group | Increment type | Increment  | Increment low bound | Forward or central switch | Multiplier (central) | Method (central) |
|-------------|----------------|------------|---------------------|---------------------------|----------------------|------------------|
| pgnam       | relative       | 1.0000E-02 | none                | switch                    | 1.500                | parabolic        |

Parameter definitions:-

| Name | Trans-formation | Change limit | Initial value | Lower bound | Upper bound |
|------|-----------------|--------------|---------------|-------------|-------------|
|------|-----------------|--------------|---------------|-------------|-------------|

|    |    |     |        |              |              |              |
|----|----|-----|--------|--------------|--------------|--------------|
| 74 | h1 | log | factor | 90.0000      | 80.0000      | 110.000      |
| 75 | s1 | log | factor | 250.000      | 1.00000      | 5000.00      |
| 76 | p1 | log | factor | 0.900000     | 0.100000     | 0.999000     |
| 77 | o1 | log | factor | 8.000000E-05 | 1.000000E-10 | 1.000000E-02 |
| 78 | h2 | log | factor | 130.000      | 120.000      | 140.000      |
| 79 | s2 | log | factor | 260.000      | 1.00000      | 5000.00      |
| 80 | p2 | log | factor | 0.900000     | 0.100000     | 0.999000     |
| 81 | o2 | log | factor | 4.000000E-05 | 1.000000E-10 | 1.000000E-02 |
| 82 | h3 | log | factor | 165.000      | 160.000      | 180.000      |
| 83 | s3 | log | factor | 260.000      | 1.00000      | 5000.00      |
| 84 | p3 | log | factor | 0.900000     | 0.100000     | 0.999000     |
| 85 | o3 | log | factor | 5.000000E-05 | 1.000000E-10 | 1.000000E-02 |

|    |      |       |         |         |       |                |
|----|------|-------|---------|---------|-------|----------------|
| 86 |      |       |         |         |       |                |
| 87 | Name | Group | Scale   | Offset  | Model | command number |
| 88 | h1   | pgnam | 1.00000 | 0.00000 | 1     |                |
| 89 | s1   | pgnam | 1.00000 | 0.00000 | 0     |                |
| 90 | p1   | pgnam | 1.00000 | 0.00000 | 1     |                |
| 91 | o1   | pgnam | 1.00000 | 0.00000 | 0     |                |
| 92 | h2   | pgnam | 1.00000 | 0.00000 | 1     |                |
| 93 | s2   | pgnam | 1.00000 | 0.00000 | 0     |                |
| 94 | p2   | pgnam | 1.00000 | 0.00000 | 1     |                |
| 95 | o2   | pgnam | 1.00000 | 0.00000 | 0     |                |
| 96 | h3   | pgnam | 1.00000 | 0.00000 | 1     |                |
| 97 | s3   | pgnam | 1.00000 | 0.00000 | 0     |                |
| 98 | p3   | pgnam | 1.00000 | 0.00000 | 1     |                |
| 99 | o3   | pgnam | 1.00000 | 0.00000 | 0     |                |

100

101

102 Prior information:-

103

104 No prior information supplied

105

106

107 Observations:-

108

|     |                  |              |            |       |
|-----|------------------|--------------|------------|-------|
| 109 | Observation name | Observation  | Weight     | Group |
| 110 | o1               | 9.793690E-08 | 0.000      | conc  |
| 111 | o2               | 9.555730E-08 | 2.9875E-34 | conc  |
| 112 | o3               | 6.909480E-08 | 2.9166E-33 | conc  |
| 113 | o4               | 3.456580E-08 | 0.000      | conc  |
| 114 | o5               | 1.385540E-08 | 0.000      | conc  |
| 115 | o6               | 2.932160E-08 | 2.2916E-32 | conc  |
| 116 | o7               | 6.577020E-08 | 2.7618E-32 | conc  |
| 117 | o8               | 7.682880E-08 | 0.000      | conc  |
| 118 | o9               | 6.670350E-08 | 0.000      | conc  |
| 119 | o10              | 6.234490E-08 | 5.2774E-31 | conc  |
| 120 | o11              | 5.799060E-08 | 0.000      | conc  |
| 121 | o12              | 4.476690E-08 | 0.000      | conc  |
| 122 | o13              | 3.367850E-08 | 2.7840E-30 | conc  |
| 123 | o14              | 3.211560E-08 | 7.0866E-30 | conc  |
| 124 | o15              | 3.667740E-08 | 0.000      | conc  |
| 125 | o16              | 4.483250E-08 | 0.000      | conc  |
| 126 | o17              | 5.451830E-08 | 8.8097E-29 | conc  |
| 127 | o18              | 5.329870E-08 | 1.7567E-29 | conc  |
| 128 | o19              | 3.170710E-08 | 0.000      | conc  |
| 129 | o20              | 1.969980E-08 | 2.2803E-28 | conc  |
| 130 | o21              | 3.595080E-08 | 1.5027E-27 | conc  |
| 131 | o22              | 4.159740E-08 | 0.000      | conc  |
| 132 | o23              | 2.288350E-08 | 0.000      | conc  |
| 133 | o24              | 1.396180E-08 | 1.3218E-26 | conc  |
| 134 | o25              | 2.130310E-08 | 1.2576E-26 | conc  |
| 135 | o26              | 2.668720E-08 | 0.000      | conc  |
| 136 | o27              | 2.834440E-08 | 0.000      | conc  |
| 137 | o28              | 3.261680E-08 | 2.8365E-25 | conc  |
| 138 | o29              | 4.429590E-08 | 0.000      | conc  |
| 139 | o30              | 5.980420E-08 | 0.000      | conc  |
| 140 | o31              | 5.733100E-08 | 1.7049E-24 | conc  |
| 141 | o32              | 3.870850E-08 | 3.5219E-24 | conc  |
| 142 | o33              | 3.932060E-08 | 0.000      | conc  |
| 143 | o34              | 6.141800E-08 | 0.000      | conc  |
| 144 | o35              | 8.121820E-08 | 6.4216E-23 | conc  |
| 145 | o36              | 9.162970E-08 | 1.8034E-22 | conc  |
| 146 | o37              | 9.354340E-08 | 2.7427E-22 | conc  |

|     |      |              |            |      |
|-----|------|--------------|------------|------|
| 147 | o38  | 8.789140E-08 | 2.8007E-22 | conc |
| 148 | o39  | 7.560540E-08 | 1.3180E-22 | conc |
| 149 | o40  | 5.780150E-08 | 0.000      | conc |
| 150 | o41  | 3.886980E-08 | 0.000      | conc |
| 151 | o42  | 2.628710E-08 | 8.5834E-22 | conc |
| 152 | o43  | 2.989340E-08 | 1.0422E-22 | conc |
| 153 | o44  | 5.157320E-08 | 0.000      | conc |
| 154 | o45  | 5.332080E-08 | 2.4642E-21 | conc |
| 155 | o46  | 2.038440E-08 | 1.4128E-20 | conc |
| 156 | o47  | 1.903840E-08 | 0.000      | conc |
| 157 | o48  | 6.196760E-08 | 0.000      | conc |
| 158 | o49  | 7.597280E-08 | 1.2914E-19 | conc |
| 159 | o50  | 5.556080E-08 | 1.1076E-19 | conc |
| 160 | o51  | 4.831800E-08 | 0.000      | conc |
| 161 | o52  | 5.189860E-08 | 0.000      | conc |
| 162 | o53  | 4.596900E-08 | 2.6974E-18 | conc |
| 163 | o54  | 3.430070E-08 | 0.000      | conc |
| 164 | o55  | 2.472200E-08 | 0.000      | conc |
| 165 | o56  | 2.023650E-08 | 1.7009E-17 | conc |
| 166 | o57  | 2.148250E-08 | 3.2382E-17 | conc |
| 167 | o58  | 2.703960E-08 | 0.000      | conc |
| 168 | o59  | 3.751750E-08 | 0.000      | conc |
| 169 | o60  | 5.294450E-08 | 4.6745E-16 | conc |
| 170 | o61  | 5.765700E-08 | 0.000      | conc |
| 171 | o62  | 4.120220E-08 | 0.000      | conc |
| 172 | o63  | 3.836340E-08 | 1.7138E-15 | conc |
| 173 | o64  | 6.394200E-08 | 7.2934E-15 | conc |
| 174 | o65  | 6.994170E-08 | 0.000      | conc |
| 175 | o66  | 4.878650E-08 | 0.000      | conc |
| 176 | o67  | 4.718890E-08 | 7.3345E-14 | conc |
| 177 | o68  | 6.046870E-08 | 4.6697E-14 | conc |
| 178 | o69  | 5.309940E-08 | 0.000      | conc |
| 179 | o70  | 3.999120E-08 | 5.7380E-14 | conc |
| 180 | o71  | 4.417600E-08 | 1.4348E-12 | conc |
| 181 | o72  | 4.504670E-08 | 0.000      | conc |
| 182 | o73  | 3.019780E-08 | 0.000      | conc |
| 183 | o74  | 2.138340E-08 | 1.0126E-11 | conc |
| 184 | o75  | 2.722030E-08 | 1.5698E-11 | conc |
| 185 | o76  | 3.698210E-08 | 0.000      | conc |
| 186 | o77  | 3.912680E-08 | 0.000      | conc |
| 187 | o78  | 2.721060E-08 | 2.5531E-10 | conc |
| 188 | o79  | 2.474320E-08 | 0.000      | conc |
| 189 | o80  | 5.070650E-08 | 0.000      | conc |
| 190 | o81  | 7.305120E-08 | 1.1428E-09 | conc |
| 191 | o82  | 7.050620E-08 | 5.3571E-09 | conc |
| 192 | o83  | 6.039960E-08 | 0.000      | conc |
| 193 | o84  | 5.758830E-08 | 0.000      | conc |
| 194 | o85  | 5.072720E-08 | 1.1595E-08 | conc |
| 195 | o86  | 3.325280E-08 | 5.4377E-08 | conc |
| 196 | o87  | 2.315410E-08 | 0.000      | conc |
| 197 | o88  | 2.704570E-08 | 0.000      | conc |
| 198 | o89  | 3.444830E-08 | 5.2756E-07 | conc |
| 199 | o90  | 5.476300E-08 | 3.7702E-07 | conc |
| 200 | o91  | 1.038760E-07 | 0.000      | conc |
| 201 | o92  | 1.349690E-07 | 2.4252E-07 | conc |
| 202 | o93  | 9.972090E-08 | 1.0565E-05 | conc |
| 203 | o94  | 4.303290E-08 | 0.000      | conc |
| 204 | o95  | 9.519600E-09 | 0.000      | conc |
| 205 | o96  | 0.00000      | 7.1661E-05 | conc |
| 206 | o97  | 2.867600E-10 | 1.1972E-04 | conc |
| 207 | o98  | 5.113690E-10 | 0.000      | conc |
| 208 | o99  | 3.620180E-10 | 0.000      | conc |
| 209 | o100 | 8.644170E-09 | 1.8620E-03 | conc |
| 210 | o101 | 1.687530E-08 | 0.000      | conc |
| 211 | o102 | 1.559690E-08 | 0.000      | conc |
| 212 | o103 | 1.561520E-08 | 7.7163E-03 | conc |
| 213 | o104 | 2.199730E-08 | 2.7854E-02 | conc |
| 214 | o105 | 2.105160E-08 | 0.000      | conc |
| 215 | o106 | 1.351390E-08 | 0.000      | conc |
| 216 | o107 | 1.636200E-08 | 0.3487     | conc |
| 217 | o108 | 2.216440E-08 | 0.9488     | conc |
| 218 | o109 | 1.374520E-08 | 1.102      | conc |
| 219 | o110 | 1.313990E-08 | 0.9934     | conc |

|     |      |              |        |      |
|-----|------|--------------|--------|------|
| 220 | o111 | 3.845720E-08 | 0.9771 | conc |
| 221 | o112 | 4.944010E-08 | 1.005  | conc |
| 222 | o113 | 2.832360E-08 | 1.004  | conc |
| 223 | o114 | 1.708140E-08 | 0.9981 | conc |
| 224 | o115 | 3.104670E-08 | 0.9993 | conc |
| 225 | o116 | 5.152090E-08 | 1.001  | conc |
| 226 | o117 | 6.025300E-08 | 1.000  | conc |
| 227 | o118 | 4.539120E-08 | 0.9999 | conc |
| 228 | o119 | 2.340680E-08 | 1.000  | conc |
| 229 | o120 | 1.412990E-08 | 1.000  | conc |
| 230 | o121 | 1.864530E-08 | 1.000  | conc |
| 231 | o122 | 2.655290E-08 | 1.000  | conc |
| 232 | o123 | 2.514160E-08 | 1.000  | conc |
| 233 | o124 | 2.011030E-08 | 1.000  | conc |
| 234 | o125 | 1.646220E-08 | 1.000  | conc |
| 235 | o126 | 1.646350E-08 | 1.000  | conc |
| 236 | o127 | 2.225790E-08 | 1.000  | conc |
| 237 | o128 | 3.508680E-08 | 1.000  | conc |
| 238 | o129 | 5.136760E-08 | 1.000  | conc |
| 239 | o130 | 6.591230E-08 | 1.000  | conc |
| 240 | o131 | 7.358170E-08 | 1.000  | conc |
| 241 | o132 | 7.271480E-08 | 1.000  | conc |
| 242 | o133 | 6.732970E-08 | 1.000  | conc |
| 243 | o134 | 6.196880E-08 | 1.000  | conc |
| 244 | o135 | 6.078950E-08 | 1.000  | conc |
| 245 | o136 | 6.429350E-08 | 1.000  | conc |
| 246 | o137 | 7.096050E-08 | 1.000  | conc |
| 247 | o138 | 7.925050E-08 | 1.000  | conc |
| 248 | o139 | 8.847530E-08 | 1.000  | conc |
| 249 | o140 | 1.002400E-07 | 1.000  | conc |
| 250 | o141 | 1.165300E-07 | 1.000  | conc |
| 251 | o142 | 1.391270E-07 | 1.000  | conc |
| 252 | o143 | 1.659020E-07 | 1.000  | conc |
| 253 | o144 | 1.912470E-07 | 1.000  | conc |
| 254 | o145 | 2.094310E-07 | 1.000  | conc |
| 255 | o146 | 2.165920E-07 | 1.000  | conc |
| 256 | o147 | 2.174470E-07 | 1.000  | conc |
| 257 | o148 | 2.191720E-07 | 1.000  | conc |
| 258 | o149 | 2.288320E-07 | 1.000  | conc |
| 259 | o150 | 2.480410E-07 | 1.000  | conc |
| 260 | o151 | 2.706290E-07 | 1.000  | conc |
| 261 | o152 | 2.898290E-07 | 1.000  | conc |
| 262 | o153 | 2.997530E-07 | 1.000  | conc |
| 263 | o154 | 3.015680E-07 | 1.000  | conc |
| 264 | o155 | 2.998420E-07 | 1.000  | conc |
| 265 | o156 | 2.991550E-07 | 1.000  | conc |
| 266 | o157 | 3.022960E-07 | 1.000  | conc |
| 267 | o158 | 3.078700E-07 | 1.000  | conc |
| 268 | o159 | 3.138870E-07 | 1.000  | conc |
| 269 | o160 | 3.184520E-07 | 1.000  | conc |
| 270 | o161 | 3.210780E-07 | 1.000  | conc |
| 271 | o162 | 3.223800E-07 | 1.000  | conc |
| 272 | o163 | 3.230020E-07 | 1.000  | conc |
| 273 | o164 | 3.235000E-07 | 1.000  | conc |
| 274 | o165 | 3.240740E-07 | 1.000  | conc |
| 275 | o166 | 3.248360E-07 | 1.000  | conc |
| 276 | o167 | 3.259000E-07 | 1.000  | conc |
| 277 | o168 | 3.273780E-07 | 1.000  | conc |
| 278 | o169 | 3.293840E-07 | 1.000  | conc |
| 279 | o170 | 3.320300E-07 | 1.000  | conc |
| 280 | o171 | 3.354300E-07 | 1.000  | conc |
| 281 | o172 | 3.396930E-07 | 1.000  | conc |
| 282 | o173 | 3.431300E-07 | 1.000  | conc |
| 283 | o174 | 3.395130E-07 | 1.000  | conc |
| 284 | o175 | 3.262010E-07 | 1.000  | conc |
| 285 | o176 | 3.068900E-07 | 1.000  | conc |
| 286 | o177 | 2.857790E-07 | 1.000  | conc |
| 287 | o178 | 2.668110E-07 | 1.000  | conc |
| 288 | o179 | 2.517910E-07 | 1.000  | conc |
| 289 | o180 | 2.414640E-07 | 1.000  | conc |
| 290 | o181 | 2.365650E-07 | 1.000  | conc |
| 291 | o182 | 2.363110E-07 | 1.000  | conc |
| 292 | o183 | 2.362840E-07 | 1.000  | conc |

|     |      |              |       |      |
|-----|------|--------------|-------|------|
| 293 | o184 | 2.315340E-07 | 1.000 | conc |
| 294 | o185 | 2.175590E-07 | 1.000 | conc |
| 295 | o186 | 1.970180E-07 | 1.000 | conc |
| 296 | o187 | 1.783120E-07 | 1.000 | conc |
| 297 | o188 | 1.700010E-07 | 1.000 | conc |
| 298 | o189 | 1.777150E-07 | 1.000 | conc |
| 299 | o190 | 1.951580E-07 | 1.000 | conc |
| 300 | o191 | 2.130090E-07 | 1.000 | conc |
| 301 | o192 | 2.220980E-07 | 1.000 | conc |
| 302 | o193 | 2.190210E-07 | 1.000 | conc |
| 303 | o194 | 2.077680E-07 | 1.000 | conc |
| 304 | o195 | 1.928170E-07 | 1.000 | conc |
| 305 | o196 | 1.781330E-07 | 1.000 | conc |
| 306 | o197 | 1.640790E-07 | 1.000 | conc |
| 307 | o198 | 1.494680E-07 | 1.000 | conc |
| 308 | o199 | 1.331190E-07 | 1.000 | conc |
| 309 | o200 | 1.157390E-07 | 1.000 | conc |
| 310 | o201 | 1.019720E-07 | 1.000 | conc |
| 311 | o202 | 9.694750E-08 | 1.000 | conc |
| 312 | o203 | 1.051370E-07 | 1.000 | conc |
| 313 | o204 | 1.223640E-07 | 1.000 | conc |
| 314 | o205 | 1.383770E-07 | 1.000 | conc |
| 315 | o206 | 1.428050E-07 | 1.000 | conc |
| 316 | o207 | 1.314920E-07 | 1.000 | conc |
| 317 | o208 | 1.220170E-07 | 1.000 | conc |
| 318 | o209 | 1.310930E-07 | 1.000 | conc |
| 319 | o210 | 1.516410E-07 | 1.000 | conc |
| 320 | o211 | 1.702820E-07 | 1.000 | conc |
| 321 | o212 | 1.738790E-07 | 1.000 | conc |
| 322 | o213 | 1.592060E-07 | 1.000 | conc |
| 323 | o214 | 1.362240E-07 | 1.000 | conc |
| 324 | o215 | 1.158070E-07 | 1.000 | conc |
| 325 | o216 | 1.075060E-07 | 1.000 | conc |
| 326 | o217 | 1.111280E-07 | 1.000 | conc |
| 327 | o218 | 1.221220E-07 | 1.000 | conc |
| 328 | o219 | 1.359230E-07 | 1.000 | conc |
| 329 | o220 | 1.490340E-07 | 1.000 | conc |
| 330 | o221 | 1.602590E-07 | 1.000 | conc |
| 331 | o222 | 1.687090E-07 | 1.000 | conc |
| 332 | o223 | 1.735440E-07 | 1.000 | conc |
| 333 | o224 | 1.746890E-07 | 1.000 | conc |
| 334 | o225 | 1.726160E-07 | 1.000 | conc |
| 335 | o226 | 1.678140E-07 | 1.000 | conc |
| 336 | o227 | 1.609850E-07 | 1.000 | conc |
| 337 | o228 | 1.536160E-07 | 1.000 | conc |
| 338 | o229 | 1.473760E-07 | 1.000 | conc |
| 339 | o230 | 1.439010E-07 | 1.000 | conc |
| 340 | o231 | 1.439110E-07 | 1.000 | conc |
| 341 | o232 | 1.470550E-07 | 1.000 | conc |
| 342 | o233 | 1.529210E-07 | 1.000 | conc |
| 343 | o234 | 1.607910E-07 | 1.000 | conc |
| 344 | o235 | 1.680200E-07 | 1.000 | conc |
| 345 | o236 | 1.712170E-07 | 1.000 | conc |
| 346 | o237 | 1.670130E-07 | 1.000 | conc |
| 347 | o238 | 1.547170E-07 | 1.000 | conc |
| 348 | o239 | 1.386780E-07 | 1.000 | conc |
| 349 | o240 | 1.238020E-07 | 1.000 | conc |
| 350 | o241 | 1.146300E-07 | 1.000 | conc |
| 351 | o242 | 1.115150E-07 | 1.000 | conc |
| 352 | o243 | 1.121430E-07 | 1.000 | conc |
| 353 | o244 | 1.141600E-07 | 1.000 | conc |
| 354 | o245 | 1.158380E-07 | 1.000 | conc |
| 355 | o246 | 1.174180E-07 | 1.000 | conc |
| 356 | o247 | 1.195250E-07 | 1.000 | conc |
| 357 | o248 | 1.227500E-07 | 1.000 | conc |
| 358 | o249 | 1.267810E-07 | 1.000 | conc |
| 359 | o250 | 1.303900E-07 | 1.000 | conc |
| 360 | o251 | 1.323070E-07 | 1.000 | conc |
| 361 | o252 | 1.312620E-07 | 1.000 | conc |
| 362 | o253 | 1.259960E-07 | 1.000 | conc |
| 363 | o254 | 1.164210E-07 | 1.000 | conc |
| 364 | o255 | 1.044990E-07 | 1.000 | conc |
| 365 | o256 | 9.240340E-08 | 1.000 | conc |

|     |      |              |       |      |
|-----|------|--------------|-------|------|
| 366 | o257 | 8.230520E-08 | 1.000 | conc |
| 367 | o258 | 7.637660E-08 | 1.000 | conc |
| 368 | o259 | 7.622740E-08 | 1.000 | conc |
| 369 | o260 | 8.043840E-08 | 1.000 | conc |
| 370 | o261 | 8.657490E-08 | 1.000 | conc |
| 371 | o262 | 9.220160E-08 | 1.000 | conc |
| 372 | o263 | 9.488300E-08 | 1.000 | conc |
| 373 | o264 | 9.228590E-08 | 1.000 | conc |
| 374 | o265 | 8.425190E-08 | 1.000 | conc |
| 375 | o266 | 7.270670E-08 | 1.000 | conc |
| 376 | o267 | 5.965960E-08 | 1.000 | conc |
| 377 | o268 | 4.711980E-08 | 1.000 | conc |
| 378 | o269 | 3.709570E-08 | 1.000 | conc |
| 379 | o270 | 3.087830E-08 | 1.000 | conc |
| 380 | o271 | 2.781440E-08 | 1.000 | conc |
| 381 | o272 | 2.692480E-08 | 1.000 | conc |
| 382 | o273 | 2.723000E-08 | 1.000 | conc |
| 383 | o274 | 2.775070E-08 | 1.000 | conc |
| 384 | o275 | 2.760460E-08 | 1.000 | conc |
| 385 | o276 | 2.676470E-08 | 1.000 | conc |
| 386 | o277 | 2.564830E-08 | 1.000 | conc |
| 387 | o278 | 2.467640E-08 | 1.000 | conc |
| 388 | o279 | 2.427000E-08 | 1.000 | conc |
| 389 | o280 | 2.484250E-08 | 1.000 | conc |
| 390 | o281 | 2.641960E-08 | 1.000 | conc |
| 391 | o282 | 2.847000E-08 | 1.000 | conc |
| 392 | o283 | 3.041950E-08 | 1.000 | conc |
| 393 | o284 | 3.169390E-08 | 1.000 | conc |
| 394 | o285 | 3.171880E-08 | 1.000 | conc |
| 395 | o286 | 3.013650E-08 | 1.000 | conc |
| 396 | o287 | 2.751750E-08 | 1.000 | conc |
| 397 | o288 | 2.468130E-08 | 1.000 | conc |
| 398 | o289 | 2.244710E-08 | 1.000 | conc |
| 399 | o290 | 2.163440E-08 | 1.000 | conc |
| 400 | o291 | 2.300960E-08 | 1.000 | conc |
| 401 | o292 | 2.652400E-08 | 1.000 | conc |
| 402 | o293 | 3.148730E-08 | 1.000 | conc |
| 403 | o294 | 3.719240E-08 | 1.000 | conc |
| 404 | o295 | 4.293170E-08 | 1.000 | conc |
| 405 | o296 | 4.799810E-08 | 1.000 | conc |
| 406 | o297 | 5.168400E-08 | 1.000 | conc |
| 407 | o298 | 5.328230E-08 | 1.000 | conc |
| 408 | o299 | 5.226800E-08 | 1.000 | conc |
| 409 | o300 | 4.918680E-08 | 1.000 | conc |
| 410 | o301 | 4.497330E-08 | 1.000 | conc |
| 411 | o302 | 4.056260E-08 | 1.000 | conc |
| 412 | o303 | 3.689010E-08 | 1.000 | conc |
| 413 | o304 | 3.486190E-08 | 1.000 | conc |
| 414 | o305 | 3.468440E-08 | 1.000 | conc |
| 415 | o306 | 3.584280E-08 | 1.000 | conc |
| 416 | o307 | 3.778920E-08 | 1.000 | conc |
| 417 | o308 | 3.997600E-08 | 1.000 | conc |
| 418 | o309 | 4.185520E-08 | 1.000 | conc |
| 419 | o310 | 4.287920E-08 | 1.000 | conc |
| 420 | o311 | 4.250540E-08 | 1.000 | conc |
| 421 | o312 | 4.056860E-08 | 1.000 | conc |
| 422 | o313 | 3.752820E-08 | 1.000 | conc |
| 423 | o314 | 3.390200E-08 | 1.000 | conc |
| 424 | o315 | 3.020810E-08 | 1.000 | conc |
| 425 | o316 | 2.696450E-08 | 1.000 | conc |
| 426 | o317 | 2.468900E-08 | 1.000 | conc |
| 427 | o318 | 2.389950E-08 | 1.000 | conc |
| 428 | o319 | 2.486570E-08 | 1.000 | conc |
| 429 | o320 | 2.718140E-08 | 1.000 | conc |
| 430 | o321 | 3.032590E-08 | 1.000 | conc |
| 431 | o322 | 3.377870E-08 | 1.000 | conc |
| 432 | o323 | 3.701890E-08 | 1.000 | conc |
| 433 | o324 | 3.952600E-08 | 1.000 | conc |
| 434 | o325 | 4.077930E-08 | 1.000 | conc |
| 435 | o326 | 4.038680E-08 | 1.000 | conc |
| 436 | o327 | 3.855690E-08 | 1.000 | conc |
| 437 | o328 | 3.567240E-08 | 1.000 | conc |
| 438 | o329 | 3.211630E-08 | 1.000 | conc |

|     |      |              |       |      |
|-----|------|--------------|-------|------|
| 439 | o330 | 2.827140E-08 | 1.000 | conc |
| 440 | o331 | 2.452070E-08 | 1.000 | conc |
| 441 | o332 | 2.124710E-08 | 1.000 | conc |
| 442 | o333 | 1.879250E-08 | 1.000 | conc |
| 443 | o334 | 1.716460E-08 | 1.000 | conc |
| 444 | o335 | 1.620760E-08 | 1.000 | conc |
| 445 | o336 | 1.576470E-08 | 1.000 | conc |
| 446 | o337 | 1.567900E-08 | 1.000 | conc |
| 447 | o338 | 1.579370E-08 | 1.000 | conc |
| 448 | o339 | 1.595200E-08 | 1.000 | conc |
| 449 | o340 | 1.600030E-08 | 1.000 | conc |
| 450 | o341 | 1.587080E-08 | 1.000 | conc |
| 451 | o342 | 1.558860E-08 | 1.000 | conc |
| 452 | o343 | 1.518340E-08 | 1.000 | conc |
| 453 | o344 | 1.468500E-08 | 1.000 | conc |
| 454 | o345 | 1.412300E-08 | 1.000 | conc |
| 455 | o346 | 1.352730E-08 | 1.000 | conc |
| 456 | o347 | 1.292740E-08 | 1.000 | conc |
| 457 | o348 | 1.234810E-08 | 1.000 | conc |
| 458 | o349 | 1.180590E-08 | 1.000 | conc |
| 459 | o350 | 1.131620E-08 | 1.000 | conc |
| 460 | o351 | 1.089450E-08 | 1.000 | conc |
| 461 | o352 | 1.055630E-08 | 1.000 | conc |
| 462 | o353 | 1.031710E-08 | 1.000 | conc |
| 463 | o354 | 1.019230E-08 | 1.000 | conc |
| 464 | o355 | 1.018390E-08 | 1.000 | conc |
| 465 | o356 | 1.025410E-08 | 1.000 | conc |
| 466 | o357 | 1.035830E-08 | 1.000 | conc |
| 467 | o358 | 1.045180E-08 | 1.000 | conc |
| 468 | o359 | 1.048990E-08 | 1.000 | conc |
| 469 | o360 | 1.042780E-08 | 1.000 | conc |
| 470 | o361 | 1.022100E-08 | 1.000 | conc |
| 471 | o362 | 9.846240E-09 | 1.000 | conc |
| 472 | o363 | 9.387050E-09 | 1.000 | conc |
| 473 | o364 | 8.959660E-09 | 1.000 | conc |
| 474 | o365 | 8.680350E-09 | 1.000 | conc |
| 475 | o366 | 8.665390E-09 | 1.000 | conc |
| 476 | o367 | 9.031040E-09 | 1.000 | conc |
| 477 | o368 | 9.893570E-09 | 1.000 | conc |
| 478 | o369 | 1.134860E-08 | 1.000 | conc |
| 479 | o370 | 1.331210E-08 | 1.000 | conc |
| 480 | o371 | 1.560750E-08 | 1.000 | conc |
| 481 | o372 | 1.805770E-08 | 1.000 | conc |
| 482 | o373 | 2.048540E-08 | 1.000 | conc |
| 483 | o374 | 2.271350E-08 | 1.000 | conc |
| 484 | o375 | 2.456470E-08 | 1.000 | conc |
| 485 | o376 | 2.587030E-08 | 1.000 | conc |
| 486 | o377 | 2.660560E-08 | 1.000 | conc |
| 487 | o378 | 2.686570E-08 | 1.000 | conc |
| 488 | o379 | 2.674930E-08 | 1.000 | conc |
| 489 | o380 | 2.635510E-08 | 1.000 | conc |
| 490 | o381 | 2.578180E-08 | 1.000 | conc |
| 491 | o382 | 2.512810E-08 | 1.000 | conc |
| 492 | o383 | 2.448710E-08 | 1.000 | conc |
| 493 | o384 | 2.393560E-08 | 1.000 | conc |
| 494 | o385 | 2.354760E-08 | 1.000 | conc |
| 495 | o386 | 2.339700E-08 | 1.000 | conc |
| 496 | o387 | 2.355770E-08 | 1.000 | conc |
| 497 | o388 | 2.410370E-08 | 1.000 | conc |
| 498 | o389 | 2.510890E-08 | 1.000 | conc |
| 499 | o390 | 2.660560E-08 | 1.000 | conc |
| 500 | o391 | 2.841940E-08 | 1.000 | conc |
| 501 | o392 | 3.031210E-08 | 1.000 | conc |
| 502 | o393 | 3.204560E-08 | 1.000 | conc |
| 503 | o394 | 3.338170E-08 | 1.000 | conc |
| 504 | o395 | 3.408220E-08 | 1.000 | conc |
| 505 | o396 | 3.390880E-08 | 1.000 | conc |
| 506 | o397 | 3.266310E-08 | 1.000 | conc |
| 507 | o398 | 3.049240E-08 | 1.000 | conc |
| 508 | o399 | 2.772300E-08 | 1.000 | conc |
| 509 | o400 | 2.468260E-08 | 1.000 | conc |
| 510 | o401 | 2.169880E-08 | 1.000 | conc |
| 511 | o402 | 1.909940E-08 | 1.000 | conc |

|     |      |              |       |      |
|-----|------|--------------|-------|------|
| 512 | o403 | 1.721200E-08 | 1.000 | conc |
| 513 | o404 | 1.634920E-08 | 1.000 | conc |
| 514 | o405 | 1.656890E-08 | 1.000 | conc |
| 515 | o406 | 1.771620E-08 | 1.000 | conc |
| 516 | o407 | 1.962940E-08 | 1.000 | conc |
| 517 | o408 | 2.214720E-08 | 1.000 | conc |
| 518 | o409 | 2.510800E-08 | 1.000 | conc |
| 519 | o410 | 2.835030E-08 | 1.000 | conc |
| 520 | o411 | 3.171240E-08 | 1.000 | conc |
| 521 | o412 | 3.502540E-08 | 1.000 | conc |
| 522 | o413 | 3.811070E-08 | 1.000 | conc |
| 523 | o414 | 4.078870E-08 | 1.000 | conc |
| 524 | o415 | 4.288030E-08 | 1.000 | conc |
| 525 | o416 | 4.420600E-08 | 1.000 | conc |
| 526 | o417 | 4.458640E-08 | 1.000 | conc |
| 527 | o418 | 4.384330E-08 | 1.000 | conc |
| 528 | o419 | 4.198300E-08 | 1.000 | conc |
| 529 | o420 | 3.941400E-08 | 1.000 | conc |
| 530 | o421 | 3.659730E-08 | 1.000 | conc |
| 531 | o422 | 3.399400E-08 | 1.000 | conc |
| 532 | o423 | 3.204760E-08 | 1.000 | conc |
| 533 | o424 | 3.086660E-08 | 1.000 | conc |
| 534 | o425 | 3.025930E-08 | 1.000 | conc |
| 535 | o426 | 3.002380E-08 | 1.000 | conc |
| 536 | o427 | 2.995800E-08 | 1.000 | conc |
| 537 | o428 | 2.985980E-08 | 1.000 | conc |
| 538 | o429 | 2.952710E-08 | 1.000 | conc |
| 539 | o430 | 2.876140E-08 | 1.000 | conc |
| 540 | o431 | 2.753560E-08 | 1.000 | conc |
| 541 | o432 | 2.606870E-08 | 1.000 | conc |
| 542 | o433 | 2.459860E-08 | 1.000 | conc |
| 543 | o434 | 2.336330E-08 | 1.000 | conc |
| 544 | o435 | 2.260070E-08 | 1.000 | conc |
| 545 | o436 | 2.254880E-08 | 1.000 | conc |
| 546 | o437 | 2.344480E-08 | 1.000 | conc |
| 547 | o438 | 2.536450E-08 | 1.000 | conc |
| 548 | o439 | 2.800460E-08 | 1.000 | conc |
| 549 | o440 | 3.100760E-08 | 1.000 | conc |
| 550 | o441 | 3.401610E-08 | 1.000 | conc |
| 551 | o442 | 3.667270E-08 | 1.000 | conc |
| 552 | o443 | 3.862000E-08 | 1.000 | conc |
| 553 | o444 | 3.950070E-08 | 1.000 | conc |
| 554 | o445 | 3.908620E-08 | 1.000 | conc |
| 555 | o446 | 3.766020E-08 | 1.000 | conc |
| 556 | o447 | 3.563300E-08 | 1.000 | conc |
| 557 | o448 | 3.341490E-08 | 1.000 | conc |
| 558 | o449 | 3.141630E-08 | 1.000 | conc |
| 559 | o450 | 3.004740E-08 | 1.000 | conc |
| 560 | o451 | 2.971880E-08 | 1.000 | conc |
| 561 | o452 | 3.075270E-08 | 1.000 | conc |
| 562 | o453 | 3.286720E-08 | 1.000 | conc |
| 563 | o454 | 3.552650E-08 | 1.000 | conc |
| 564 | o455 | 3.819390E-08 | 1.000 | conc |
| 565 | o456 | 4.033280E-08 | 1.000 | conc |
| 566 | o457 | 4.140650E-08 | 1.000 | conc |
| 567 | o458 | 4.087830E-08 | 1.000 | conc |
| 568 | o459 | 3.826280E-08 | 1.000 | conc |
| 569 | o460 | 3.372330E-08 | 1.000 | conc |
| 570 | o461 | 2.786850E-08 | 1.000 | conc |
| 571 | o462 | 2.131620E-08 | 1.000 | conc |
| 572 | o463 | 1.468380E-08 | 1.000 | conc |
| 573 | o464 | 8.588990E-09 | 1.000 | conc |
| 574 | o465 | 3.649360E-09 | 1.000 | conc |
| 575 | o466 | 4.677260E-10 | 1.000 | conc |
| 576 | o467 | 0.00000      | 1.000 | conc |
| 577 | o468 | 0.00000      | 1.000 | conc |
| 578 | o469 | 1.626740E-09 | 1.000 | conc |
| 579 | o470 | 4.693200E-09 | 1.000 | conc |
| 580 | o471 | 8.644330E-09 | 1.000 | conc |
| 581 | o472 | 1.320690E-08 | 1.000 | conc |
| 582 | o473 | 1.810750E-08 | 1.000 | conc |
| 583 | o474 | 2.306840E-08 | 1.000 | conc |
| 584 | o475 | 2.780330E-08 | 1.000 | conc |



|     |      |              |       |      |
|-----|------|--------------|-------|------|
| 585 | o476 | 3.202510E-08 | 1.000 | conc |
| 586 | o477 | 3.544690E-08 | 1.000 | conc |
| 587 | o478 | 3.778170E-08 | 1.000 | conc |
| 588 | o479 | 3.874230E-08 | 1.000 | conc |
| 589 | o480 | 3.804200E-08 | 1.000 | conc |
| 590 | o481 | 3.556310E-08 | 1.000 | conc |
| 591 | o482 | 3.168540E-08 | 1.000 | conc |
| 592 | o483 | 2.688000E-08 | 1.000 | conc |
| 593 | o484 | 2.161760E-08 | 1.000 | conc |
| 594 | o485 | 1.636920E-08 | 1.000 | conc |
| 595 | o486 | 1.160560E-08 | 1.000 | conc |
| 596 | o487 | 7.797780E-09 | 1.000 | conc |
| 597 | o488 | 5.321320E-09 | 1.000 | conc |
| 598 | o489 | 4.072160E-09 | 1.000 | conc |
| 599 | o490 | 3.795720E-09 | 1.000 | conc |
| 600 | o491 | 4.237380E-09 | 1.000 | conc |
| 601 | o492 | 5.142490E-09 | 1.000 | conc |
| 602 | o493 | 6.256440E-09 | 1.000 | conc |
| 603 | o494 | 7.324600E-09 | 1.000 | conc |
| 604 | o495 | 8.113290E-09 | 1.000 | conc |
| 605 | o496 | 8.575080E-09 | 1.000 | conc |
| 606 | o497 | 8.760030E-09 | 1.000 | conc |
| 607 | o498 | 8.719080E-09 | 1.000 | conc |
| 608 | o499 | 8.503150E-09 | 1.000 | conc |
| 609 | o500 | 8.163170E-09 | 1.000 | conc |

610  
611

612 Control settings:-

613

|     |  |   |             |
|-----|--|---|-------------|
| 614 | Initial lambda   | : | 10.000      |
| 615 | Lambda adjustment factor                                     | : | 2.0000      |
| 616 | Sufficient new/old phi ratio per optimisation iteration      | : | 0.30000     |
| 617 | Limiting relative phi reduction between lambdas              | : | 1.00000E-02 |
| 618 | Maximum trial lambdas per iteration                          | : | 8           |
| 619 | Forgive model run failure during lamda testing               | : | yes         |
| 620 | Forgive model run failure during Jacobian runs               | : | yes         |
| 621 |  |   |             |
| 622 | Perform Broyden's update of Jacobian matrix                  | : | no          |
| 623 | Undertake observation re-referencing                         | : | no          |
| 624 |  |   |             |
| 625 | Maximum factor parameter change (factor-limited changes)     | : | 10.000      |
| 626 | Maximum relative parameter change (relative-limited changes) | : | na          |
| 627 | Fraction of initial parameter values used in computing       |   |             |
| 628 | change limit for near-zero parameters                        | : | 1.00000E-03 |
| 629 | Allow bending of parameter upgrade vector                    | : | no          |
| 630 | Allow parameters to stick to their bounds                    | : | no          |
| 631 |  |   |             |
| 632 | Relative phi reduction below which to begin use of           |   |             |
| 633 | central derivatives  | : | 0.10000     |
| 634 | Iteration at which to first consider derivatives switch      | : | 1           |
| 635 |  |   |             |
| 636 | Relative phi reduction indicating convergence                | : | 0.50000E-02 |
| 637 | Number of phi values required within this range              | : | 4           |
| 638 | Maximum number of consecutive failures to lower phi          | : | 4           |
| 639 | Minimal relative parameter change indicating convergence     | : | 0.50000E-02 |
| 640 | Number of consecutive iterations with minimal param change   | : | 4           |
| 641 | Maximum number of optimisation iterations                    | : | 200         |
| 642 |  |   |             |
| 643 | Attempt automatic user intervention                          | : | no          |
| 644 |  |   |             |
| 645 | Attempt reuse of parameter sensitivities                     | : | no          |
| 646 |  |   |             |
| 647 | Scale parameters by their bounds                             | : | yes         |

648  
649

650 File saving options: -

651

|     |                         |   |     |
|-----|-------------------------|---|-----|
| 652 | Save best JCO file      | : | yes |
| 653 | Save multiple JCO files | : | no  |
| 654 | Save multiple REI files | : | no  |
| 655 | Save multiple PAR files | : | yes |

656  
657

# OPTIMISATION RECORD

## INITIAL CONDITIONS:

Sum of squared weighted residuals (ie phi) = 1.98446E-13

### Current parameter values

|    |              |
|----|--------------|
| h1 | 90.0000      |
| s1 | 250.000      |
| p1 | 0.900000     |
| o1 | 8.000000E-05 |
| h2 | 130.000      |
| s2 | 260.000      |
| p2 | 0.900000     |
| o2 | 4.000000E-05 |
| h3 | 165.000      |
| s3 | 260.000      |
| p3 | 0.900000     |
| o3 | 5.000000E-05 |

OPTIMISATION ITERATION NO. : 1

Model calls so far : 1

Derivative model calls so far : 0

Starting phi for this iteration: 1.98446E-13

Lambda = 10.000 ----->

Phi = 1.95988E-13 ( 0.988 of starting phi)

Lambda = 5.0000 ----->

Phi = 1.95988E-13 ( 0.988 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0100

Lowest phi this iteration: 1.95988E-13

Relative phi reduction between optimisation iterations less than 0.1000

Switch to higher order derivatives calculation

### Current parameter values

|    |              |
|----|--------------|
| h1 | 90.0054      |
| s1 | 248.315      |
| p1 | 0.893119     |
| o1 | 8.049647E-05 |
| h2 | 130.000      |
| s2 | 260.285      |
| p2 | 0.900623     |
| o2 | 3.995065E-05 |
| h3 | 165.000      |
| s3 | 259.831      |
| p3 | 0.900228     |
| o3 | 5.011740E-05 |

### Previous parameter values

|    |              |
|----|--------------|
| h1 | 90.0000      |
| s1 | 250.000      |
| p1 | 0.900000     |
| o1 | 8.000000E-05 |
| h2 | 130.000      |
| s2 | 260.000      |
| p2 | 0.900000     |
| o2 | 4.000000E-05 |
| h3 | 165.000      |
| s3 | 260.000      |
| p3 | 0.900000     |
| o3 | 5.000000E-05 |

Maximum factor change: 1.008 ["p1"]

Maximum relative change: 7.6459E-03 ["p1"]

OPTIMISATION ITERATION NO. : 2

Model calls so far : 9

Derivative model calls so far : 1

Starting phi for this iteration: 1.95988E-13

Lambda = 5.0000 ----->

Phi = 1.95952E-13 ( 1.000 of starting phi)

Lambda = 2.5000 ----->

Phi = 1.95952E-13 ( 1.000 of starting phi)

No more lambdas: relative phi reduction between lambdas less than 0.0100

Lowest phi this iteration: 1.95952E-13

### Current parameter values

|    |              |
|----|--------------|
| h1 | 90.0072      |
| s1 | 247.963      |
| p1 | 0.892184     |
| o1 | 8.054990E-05 |

### Previous parameter values

|    |              |
|----|--------------|
| h1 | 90.0054      |
| s1 | 248.315      |
| p1 | 0.893119     |
| o1 | 8.049647E-05 |

```

731      h2          129.999          h2          130.000
732      s2          260.191          s2          260.285
733      p2          0.900733          p2          0.900623
734      o2          3.992553E-05          o2          3.995065E-05
735      h3          165.001          h3          165.000
736      s3          259.293          s3          259.831
737      p3          0.900920          p3          0.900228
738      o3          5.058311E-05          o3          5.011740E-05
739      Maximum factor change: 1.009 ["o3"]
740      Maximum relative change: 9.2924E-03 ["o3"]
741
742
743      OPTIMISATION ITERATION NO.          : 3
744      Model calls so far          : 23
745      Derivative model calls so far : 2
746      Starting phi for this iteration: 1.95952E-13
747
748      Lambda = 2.5000 ----->
749      Phi = 1.95908E-13 ( 1.000 of starting phi)
750
751      Lambda = 1.2500 ----->
752      Phi = 1.95908E-13 ( 1.000 of starting phi)
753
754      No more lambdas: relative phi reduction between lambdas less than 0.0100
755      Lowest phi this iteration: 1.95908E-13
756
757      Current parameter values          Previous parameter values
758      h1          90.0080          h1          90.0072
759      s1          248.131          s1          247.963
760      p1          0.893152          p1          0.892184
761      o1          8.046042E-05          o1          8.054990E-05
762      h2          129.999          h2          129.999
763      s2          259.967          s2          260.191
764      p2          0.900518          p2          0.900733
765      o2          3.989134E-05          o2          3.992553E-05
766      h3          165.002          h3          165.001
767      s3          258.765          s3          259.293
768      p3          0.901591          p3          0.900920
769      o3          5.106194E-05          o3          5.058311E-05
770      Maximum factor change: 1.009 ["o3"]
771      Maximum relative change: 9.4663E-03 ["o3"]
772
773
774      OPTIMISATION ITERATION NO.          : 4
775      Model calls so far          : 37
776      Derivative model calls so far : 3
777      Starting phi for this iteration: 1.95908E-13
778
779      Lambda = 1.2500 ----->
780      Phi = 1.95875E-13 ( 1.000 of starting phi)
781
782      Lambda = 0.62500 ----->
783      Phi = 1.95875E-13 ( 1.000 of starting phi)
784
785      No more lambdas: relative phi reduction between lambdas less than 0.0100
786      Lowest phi this iteration: 1.95875E-13
787
788      Current parameter values          Previous parameter values
789      h1          90.0097          h1          90.0080
790      s1          247.777          s1          248.131
791      p1          0.892252          p1          0.893152
792      o1          8.051378E-05          o1          8.046042E-05
793      h2          129.998          h2          129.999
794      s2          259.897          s2          259.967
795      p2          0.900710          p2          0.900518
796      o2          3.987043E-05          o2          3.989134E-05
797      h3          165.002          h3          165.002
798      s3          258.298          s3          258.765
799      p3          0.902186          p3          0.901591
800      o3          5.147327E-05          o3          5.106194E-05
801      Maximum factor change: 1.008 ["o3"]
802      Maximum relative change: 8.0555E-03 ["o3"]
803

```

804 Optimisation complete: the 4 lowest phi's are within a relative distance  
 805 of eachother of 5.000E-03  
 806 Total model calls: 51  
 807  
 808 The model has been run one final time using best parameters.  
 809 Thus all model input files contain best parameter values, and model  
 810 output files contain model results based on these parameters.  
 811

# 813 OPTIMISATION RESULTS

815 Covariance matrix and parameter confidence intervals cannot be determined:-  
 816 Memory conservation is operative so that covariance matrix is not calculated.  
 817

## 819 Parameters ----->

| 821 Parameter | Estimated value |
|---------------|-----------------|
| 822 h1        | 90.0097         |
| 823 s1        | 247.777         |
| 824 p1        | 0.892252        |
| 825 o1        | 8.051378E-05    |
| 826 h2        | 129.998         |
| 827 s2        | 259.897         |
| 828 p2        | 0.900710        |
| 829 o2        | 3.987043E-05    |
| 830 h3        | 165.002         |
| 831 s3        | 258.298         |
| 832 p3        | 0.902186        |
| 833 o3        | 5.147327E-05    |

835 See file mfit.sen for parameter sensitivities.  
 836

## 838 Observations ----->

| 840 Observation | Measured value | Calculated value | Residual     | Weight     | Group |
|-----------------|----------------|------------------|--------------|------------|-------|
| 841 o1          | 9.793690E-08   | 0.00000          | 9.793690E-08 | 0.000      |       |
| 842 conc        |                |                  |              |            |       |
| 843 o2          | 9.555730E-08   | 0.00000          | 9.555730E-08 | 2.9875E-34 |       |
| 844 conc        |                |                  |              |            |       |
| 845 o3          | 6.909480E-08   | 0.00000          | 6.909480E-08 | 2.9166E-33 |       |
| 846 conc        |                |                  |              |            |       |
| 847 o4          | 3.456580E-08   | 0.00000          | 3.456580E-08 | 0.000      |       |
| 848 conc        |                |                  |              |            |       |
| 849 o5          | 1.385540E-08   | 0.00000          | 1.385540E-08 | 0.000      |       |
| 850 conc        |                |                  |              |            |       |
| 851 o6          | 2.932160E-08   | 0.00000          | 2.932160E-08 | 2.2916E-32 |       |
| 852 conc        |                |                  |              |            |       |
| 853 o7          | 6.577020E-08   | 0.00000          | 6.577020E-08 | 2.7618E-32 |       |
| 854 conc        |                |                  |              |            |       |
| 855 o8          | 7.682880E-08   | 0.00000          | 7.682880E-08 | 0.000      |       |
| 856 conc        |                |                  |              |            |       |
| 857 o9          | 6.670350E-08   | 0.00000          | 6.670350E-08 | 0.000      |       |
| 858 conc        |                |                  |              |            |       |
| 859 o10         | 6.234490E-08   | 0.00000          | 6.234490E-08 | 5.2774E-31 |       |
| conc            |                |                  |              |            |       |
| o11             | 5.799060E-08   | 5.434722-322     | 5.799060E-08 | 0.000      |       |
| conc            |                |                  |              |            |       |
| o12             | 4.476690E-08   | 2.061434-293     | 4.476690E-08 | 0.000      |       |
| conc            |                |                  |              |            |       |
| o13             | 3.367850E-08   | 5.261114-269     | 3.367850E-08 | 2.7840E-30 |       |
| conc            |                |                  |              |            |       |
| o14             | 3.211560E-08   | 6.347935-248     | 3.211560E-08 | 7.0866E-30 |       |
| conc            |                |                  |              |            |       |
| o15             | 3.667740E-08   | 1.551079-229     | 3.667740E-08 | 0.000      |       |
| conc            |                |                  |              |            |       |
| o16             | 4.483250E-08   | 2.324796-213     | 4.483250E-08 | 0.000      |       |
| conc            |                |                  |              |            |       |
| o17             | 5.451830E-08   | 5.046382-199     | 5.451830E-08 | 8.8097E-29 |       |
| conc            |                |                  |              |            |       |
| o18             | 5.329870E-08   | 3.119588-186     | 5.329870E-08 | 1.7567E-29 |       |

|     |             |              |              |              |            |
|-----|-------------|--------------|--------------|--------------|------------|
| 860 | conc<br>o19 | 3.170710E-08 | 9.420147-175 | 3.170710E-08 | 0.000      |
| 861 | conc<br>o20 | 1.969980E-08 | 2.148331-164 | 1.969980E-08 | 2.2803E-28 |
| 862 | conc<br>o21 | 3.595080E-08 | 5.281148-155 | 3.595080E-08 | 1.5027E-27 |
| 863 | conc<br>o22 | 4.159740E-08 | 1.876387-146 | 4.159740E-08 | 0.000      |
| 864 | conc<br>o23 | 2.288350E-08 | 1.229837-138 | 2.288350E-08 | 0.000      |
| 865 | conc<br>o24 | 1.396180E-08 | 1.824607-131 | 1.396180E-08 | 1.3218E-26 |
| 866 | conc<br>o25 | 2.130310E-08 | 7.283986-125 | 2.130310E-08 | 1.2576E-26 |
| 867 | conc<br>o26 | 2.668720E-08 | 9.063933-119 | 2.668720E-08 | 0.000      |
| 868 | conc<br>o27 | 2.834440E-08 | 3.987380-113 | 2.834440E-08 | 0.000      |
| 869 | conc<br>o28 | 3.261680E-08 | 6.911307-108 | 3.261680E-08 | 2.8365E-25 |
| 870 | conc<br>o29 | 4.429590E-08 | 5.184299-103 | 4.429590E-08 | 0.000      |
| 871 | conc<br>o30 | 5.980420E-08 | 1.826154E-98 | 5.980420E-08 | 0.000      |
| 872 | conc<br>o31 | 5.733100E-08 | 3.244141E-94 | 5.733100E-08 | 1.7049E-24 |
| 873 | conc<br>o32 | 3.870850E-08 | 3.094514E-90 | 3.870850E-08 | 3.5219E-24 |
| 874 | conc<br>o33 | 3.932060E-08 | 1.674977E-86 | 3.932060E-08 | 0.000      |
| 875 | conc<br>o34 | 6.141800E-08 | 5.402343E-83 | 6.141800E-08 | 0.000      |
| 876 | conc<br>o35 | 8.121820E-08 | 1.084358E-79 | 8.121820E-08 | 6.4216E-23 |
| 877 | conc<br>o36 | 9.162970E-08 | 1.407956E-76 | 9.162970E-08 | 1.8034E-22 |
| 878 | conc<br>o37 | 9.354340E-08 | 1.224224E-73 | 9.354340E-08 | 2.7427E-22 |
| 879 | conc<br>o38 | 8.789140E-08 | 7.353036E-71 | 8.789140E-08 | 2.8007E-22 |
| 880 | conc<br>o39 | 7.560540E-08 | 3.137111E-68 | 7.560540E-08 | 1.3180E-22 |
| 881 | conc<br>o40 | 5.780150E-08 | 9.749559E-66 | 5.780150E-08 | 0.000      |
| 882 | conc<br>o41 | 3.886980E-08 | 2.257974E-63 | 3.886980E-08 | 0.000      |
| 883 | conc<br>o42 | 2.628710E-08 | 3.978274E-61 | 2.628710E-08 | 8.5834E-22 |
| 884 | conc<br>o43 | 2.989340E-08 | 5.433201E-59 | 2.989340E-08 | 1.0422E-22 |
| 885 | conc<br>o44 | 5.157320E-08 | 5.850841E-57 | 5.157320E-08 | 0.000      |
| 886 | conc<br>o45 | 5.332080E-08 | 5.046036E-55 | 5.332080E-08 | 2.4642E-21 |
| 887 | conc<br>o46 | 2.038440E-08 | 3.535420E-53 | 2.038440E-08 | 1.4128E-20 |
| 888 | conc<br>o47 | 1.903840E-08 | 2.038738E-51 | 1.903840E-08 | 0.000      |
| 889 | conc<br>o48 | 6.196760E-08 | 9.793032E-50 | 6.196760E-08 | 0.000      |
| 890 | conc<br>o49 | 7.597280E-08 | 3.961830E-48 | 7.597280E-08 | 1.2914E-19 |
| 891 | conc<br>o50 | 5.556080E-08 | 1.363664E-46 | 5.556080E-08 | 1.1076E-19 |
| 892 | conc<br>o51 | 4.831800E-08 | 4.031083E-45 | 4.831800E-08 | 0.000      |
| 893 | conc<br>o52 | 5.189860E-08 | 1.032284E-43 | 5.189860E-08 | 0.000      |
| 894 | conc<br>o53 | 4.596900E-08 | 2.308455E-42 | 4.596900E-08 | 2.6974E-18 |
| 895 | conc<br>o54 | 3.430070E-08 | 4.541662E-41 | 3.430070E-08 | 0.000      |

|     |             |              |              |              |            |
|-----|-------------|--------------|--------------|--------------|------------|
| 896 | o55         | 2.472200E-08 | 7.915439E-40 | 2.472200E-08 | 0.000      |
| 897 | conc<br>o56 | 2.023650E-08 | 1.229946E-38 | 2.023650E-08 | 1.7009E-17 |
| 898 | conc<br>o57 | 2.148250E-08 | 1.714115E-37 | 2.148250E-08 | 3.2382E-17 |
| 899 | conc<br>o58 | 2.703960E-08 | 2.154523E-36 | 2.703960E-08 | 0.000      |
| 900 | conc<br>o59 | 3.751750E-08 | 2.455123E-35 | 3.751750E-08 | 0.000      |
| 901 | conc<br>o60 | 5.294450E-08 | 2.548657E-34 | 5.294450E-08 | 4.6745E-16 |
| 902 | conc<br>o61 | 5.765700E-08 | 2.421220E-33 | 5.765700E-08 | 0.000      |
| 903 | conc<br>o62 | 4.120220E-08 | 2.113903E-32 | 4.120220E-08 | 0.000      |
| 904 | conc<br>o63 | 3.836340E-08 | 1.702908E-31 | 3.836340E-08 | 1.7138E-15 |
| 905 | conc<br>o64 | 6.394200E-08 | 1.270497E-30 | 6.394200E-08 | 7.2934E-15 |
| 906 | conc<br>o65 | 6.994170E-08 | 8.809576E-30 | 6.994170E-08 | 0.000      |
| 907 | conc<br>o66 | 4.878650E-08 | 5.695946E-29 | 4.878650E-08 | 0.000      |
| 908 | conc<br>o67 | 4.718890E-08 | 3.444712E-28 | 4.718890E-08 | 7.3345E-14 |
| 909 | conc<br>o68 | 6.046870E-08 | 1.954269E-27 | 6.046870E-08 | 4.6697E-14 |
| 910 | conc<br>o69 | 5.309940E-08 | 1.042932E-26 | 5.309940E-08 | 0.000      |
| 911 | conc<br>o70 | 3.999120E-08 | 5.249226E-26 | 3.999120E-08 | 5.7380E-14 |
| 912 | conc<br>o71 | 4.417600E-08 | 2.497857E-25 | 4.417600E-08 | 1.4348E-12 |
| 913 | conc<br>o72 | 4.504670E-08 | 1.126365E-24 | 4.504670E-08 | 0.000      |
| 914 | conc<br>o73 | 3.019780E-08 | 4.823719E-24 | 3.019780E-08 | 0.000      |
| 915 | conc<br>o74 | 2.138340E-08 | 1.965971E-23 | 2.138340E-08 | 1.0126E-11 |
| 916 | conc<br>o75 | 2.722030E-08 | 7.640435E-23 | 2.722030E-08 | 1.5698E-11 |
| 917 | conc<br>o76 | 3.698210E-08 | 2.836701E-22 | 3.698210E-08 | 0.000      |
| 918 | conc<br>o77 | 3.912680E-08 | 1.007931E-21 | 3.912680E-08 | 0.000      |
| 919 | conc<br>o78 | 2.721060E-08 | 3.433196E-21 | 2.721060E-08 | 2.5531E-10 |
| 920 | conc<br>o79 | 2.474320E-08 | 1.122815E-20 | 2.474320E-08 | 0.000      |
| 921 | conc<br>o80 | 5.070650E-08 | 3.531164E-20 | 5.070650E-08 | 0.000      |
| 922 | conc<br>o81 | 7.305120E-08 | 1.069430E-19 | 7.305120E-08 | 1.1428E-09 |
| 923 | conc<br>o82 | 7.050620E-08 | 3.123256E-19 | 7.050620E-08 | 5.3571E-09 |
| 924 | conc<br>o83 | 6.039960E-08 | 8.807440E-19 | 6.039960E-08 | 0.000      |
| 925 | conc<br>o84 | 5.758830E-08 | 2.401148E-18 | 5.758830E-08 | 0.000      |
| 926 | conc<br>o85 | 5.072720E-08 | 6.336222E-18 | 5.072720E-08 | 1.1595E-08 |
| 927 | conc<br>o86 | 3.325280E-08 | 1.620224E-17 | 3.325280E-08 | 5.4377E-08 |
| 928 | conc<br>o87 | 2.315410E-08 | 4.019034E-17 | 2.315410E-08 | 0.000      |
| 929 | conc<br>o88 | 2.704570E-08 | 9.680952E-17 | 2.704570E-08 | 0.000      |
| 930 | conc<br>o89 | 3.444830E-08 | 2.266689E-16 | 3.444830E-08 | 5.2756E-07 |
| 931 | conc<br>o90 | 5.476300E-08 | 5.163597E-16 | 5.476300E-08 | 3.7702E-07 |
| 932 | conc<br>o91 | 1.038760E-07 | 1.145487E-15 | 1.038760E-07 | 0.000      |

|     |              |              |              |               |            |
|-----|--------------|--------------|--------------|---------------|------------|
| 933 | conc<br>o92  | 1.349690E-07 | 2.476737E-15 | 1.349690E-07  | 2.4252E-07 |
| 934 | conc<br>o93  | 9.972090E-08 | 5.223721E-15 | 9.972089E-08  | 1.0565E-05 |
| 935 | conc<br>o94  | 4.303290E-08 | 1.075557E-14 | 4.303289E-08  | 0.000      |
| 936 | conc<br>o95  | 9.519600E-09 | 2.163563E-14 | 9.519578E-09  | 0.000      |
| 937 | conc<br>o96  | 0.00000      | 4.255038E-14 | -4.255038E-14 | 7.1661E-05 |
| 938 | conc<br>o97  | 2.867600E-10 | 8.187245E-14 | 2.866781E-10  | 1.1972E-04 |
| 939 | conc<br>o98  | 5.113690E-10 | 1.542279E-13 | 5.112148E-10  | 0.000      |
| 940 | conc<br>o99  | 3.620180E-10 | 2.846149E-13 | 3.617334E-10  | 0.000      |
| 941 | conc<br>o100 | 8.644170E-09 | 5.148604E-13 | 8.643655E-09  | 1.8620E-03 |
| 942 | conc<br>o101 | 1.687530E-08 | 9.135156E-13 | 1.687439E-08  | 0.000      |
| 943 | conc<br>o102 | 1.559690E-08 | 1.590685E-12 | 1.559531E-08  | 0.000      |
| 944 | conc<br>o103 | 1.561520E-08 | 2.719770E-12 | 1.561248E-08  | 7.7163E-03 |
| 945 | conc<br>o104 | 2.199730E-08 | 4.568656E-12 | 2.199273E-08  | 2.7854E-02 |
| 946 | conc<br>o105 | 2.105160E-08 | 7.543512E-12 | 2.104406E-08  | 0.000      |
| 947 | conc<br>o106 | 1.351390E-08 | 1.224897E-11 | 1.350165E-08  | 0.000      |
| 948 | conc<br>o107 | 1.636200E-08 | 1.956907E-11 | 1.634243E-08  | 0.3487     |
| 949 | conc<br>o108 | 2.216440E-08 | 3.077393E-11 | 2.213363E-08  | 0.9488     |
| 950 | conc<br>o109 | 1.374520E-08 | 4.765706E-11 | 1.369754E-08  | 1.102      |
| 951 | conc<br>o110 | 1.313990E-08 | 7.270866E-11 | 1.306719E-08  | 0.9934     |
| 952 | conc<br>o111 | 3.845720E-08 | 1.093292E-10 | 3.834787E-08  | 0.9771     |
| 953 | conc<br>o112 | 4.944010E-08 | 1.620868E-10 | 4.927801E-08  | 1.005      |
| 954 | conc<br>o113 | 2.832360E-08 | 2.370200E-10 | 2.808658E-08  | 1.004      |
| 955 | conc<br>o114 | 1.708140E-08 | 3.419853E-10 | 1.673941E-08  | 0.9981     |
| 956 | conc<br>o115 | 3.104670E-08 | 4.870439E-10 | 3.055966E-08  | 0.9993     |
| 957 | conc<br>o116 | 5.152090E-08 | 6.848819E-10 | 5.083602E-08  | 1.001      |
| 958 | conc<br>o117 | 6.025300E-08 | 9.512475E-10 | 5.930175E-08  | 1.000      |
| 959 | conc<br>o118 | 4.539120E-08 | 1.305391E-09 | 4.408581E-08  | 0.9999     |
| 960 | conc<br>o119 | 2.340680E-08 | 1.770479E-09 | 2.163632E-08  | 1.000      |
| 961 | conc<br>o120 | 1.412990E-08 | 2.373967E-09 | 1.175593E-08  | 1.000      |
| 962 | conc<br>o121 | 1.864530E-08 | 3.147880E-09 | 1.549742E-08  | 1.000      |
| 963 | conc<br>o122 | 2.655290E-08 | 4.128982E-09 | 2.242392E-08  | 1.000      |
| 964 | conc<br>o123 | 2.514160E-08 | 5.358803E-09 | 1.978280E-08  | 1.000      |
| 965 | conc<br>o124 | 2.011030E-08 | 6.883467E-09 | 1.322683E-08  | 1.000      |
| 966 | conc<br>o125 | 1.646220E-08 | 8.753315E-09 | 7.708885E-09  | 1.000      |
| 967 | conc<br>o126 | 1.646350E-08 | 1.102229E-08 | 5.441208E-09  | 1.000      |
| 968 | conc<br>o127 | 2.225790E-08 | 1.374707E-08 | 8.510827E-09  | 1.000      |

|      |              |              |              |               |       |
|------|--------------|--------------|--------------|---------------|-------|
| 969  | o128<br>conc | 3.508680E-08 | 1.698594E-08 | 1.810086E-08  | 1.000 |
| 970  | o129<br>conc | 5.136760E-08 | 2.079739E-08 | 3.057021E-08  | 1.000 |
| 971  | o130<br>conc | 6.591230E-08 | 2.523856E-08 | 4.067374E-08  | 1.000 |
| 972  | o131<br>conc | 7.358170E-08 | 3.036343E-08 | 4.321827E-08  | 1.000 |
| 973  | o132<br>conc | 7.271480E-08 | 3.622086E-08 | 3.649394E-08  | 1.000 |
| 974  | o133<br>conc | 6.732970E-08 | 4.285262E-08 | 2.447708E-08  | 1.000 |
| 975  | o134<br>conc | 6.196880E-08 | 5.029138E-08 | 1.167742E-08  | 1.000 |
| 976  | o135<br>conc | 6.078950E-08 | 5.855879E-08 | 2.230709E-09  | 1.000 |
| 977  | o136<br>conc | 6.429350E-08 | 6.766368E-08 | -3.370181E-09 | 1.000 |
| 978  | o137<br>conc | 7.096050E-08 | 7.760058E-08 | -6.640080E-09 | 1.000 |
| 979  | o138<br>conc | 7.925050E-08 | 8.834850E-08 | -9.097998E-09 | 1.000 |
| 980  | o139<br>conc | 8.847530E-08 | 9.987012E-08 | -1.139482E-08 | 1.000 |
| 981  | o140<br>conc | 1.002400E-07 | 1.121115E-07 | -1.187146E-08 | 1.000 |
| 982  | o141<br>conc | 1.165300E-07 | 1.250019E-07 | -8.471948E-09 | 1.000 |
| 983  | o142<br>conc | 1.391270E-07 | 1.384551E-07 | 6.719474E-10  | 1.000 |
| 984  | o143<br>conc | 1.659020E-07 | 1.523694E-07 | 1.353259E-08  | 1.000 |
| 985  | o144<br>conc | 1.912470E-07 | 1.666304E-07 | 2.461660E-08  | 1.000 |
| 986  | o145<br>conc | 2.094310E-07 | 1.811122E-07 | 2.831884E-08  | 1.000 |
| 987  | o146<br>conc | 2.165920E-07 | 1.956800E-07 | 2.091203E-08  | 1.000 |
| 988  | o147<br>conc | 2.174470E-07 | 2.101930E-07 | 7.254047E-09  | 1.000 |
| 989  | o148<br>conc | 2.191720E-07 | 2.245070E-07 | -5.334960E-09 | 1.000 |
| 990  | o149<br>conc | 2.288320E-07 | 2.384776E-07 | -9.645570E-09 | 1.000 |
| 991  | o150<br>conc | 2.480410E-07 | 2.519631E-07 | -3.922115E-09 | 1.000 |
| 992  | o151<br>conc | 2.706290E-07 | 2.648276E-07 | 5.801377E-09  | 1.000 |
| 993  | o152<br>conc | 2.898290E-07 | 2.769436E-07 | 1.288542E-08  | 1.000 |
| 994  | o153<br>conc | 2.997530E-07 | 2.881944E-07 | 1.155856E-08  | 1.000 |
| 995  | o154<br>conc | 3.015680E-07 | 2.984768E-07 | 3.091196E-09  | 1.000 |
| 996  | o155<br>conc | 2.998420E-07 | 3.077022E-07 | -7.860232E-09 | 1.000 |
| 997  | o156<br>conc | 2.991550E-07 | 3.157986E-07 | -1.664361E-08 | 1.000 |
| 998  | o157<br>conc | 3.022960E-07 | 3.227111E-07 | -2.041507E-08 | 1.000 |
| 999  | o158<br>conc | 3.078700E-07 | 3.284025E-07 | -2.053249E-08 | 1.000 |
| 1000 | o159<br>conc | 3.138870E-07 | 3.328535E-07 | -1.896653E-08 | 1.000 |
| 1001 | o160<br>conc | 3.184520E-07 | 3.360622E-07 | -1.761019E-08 | 1.000 |
| 1002 | o161<br>conc | 3.210780E-07 | 3.380431E-07 | -1.696514E-08 | 1.000 |
| 1003 | o162<br>conc | 3.223800E-07 | 3.388265E-07 | -1.644650E-08 | 1.000 |
| 1004 | o163<br>conc | 3.230020E-07 | 3.384565E-07 | -1.545455E-08 | 1.000 |
| 1005 | o164         | 3.235000E-07 | 3.369901E-07 | -1.349006E-08 | 1.000 |



|      |              |              |              |               |       |
|------|--------------|--------------|--------------|---------------|-------|
| 1006 | conc<br>o165 | 3.240740E-07 | 3.344945E-07 | -1.042053E-08 | 1.000 |
| 1007 | conc<br>o166 | 3.248360E-07 | 3.310463E-07 | -6.210346E-09 | 1.000 |
| 1008 | conc<br>o167 | 3.259000E-07 | 3.267288E-07 | -8.288124E-10 | 1.000 |
| 1009 | conc<br>o168 | 3.273780E-07 | 3.216303E-07 | 5.747707E-09  | 1.000 |
| 1010 | conc<br>o169 | 3.293840E-07 | 3.158424E-07 | 1.354164E-08  | 1.000 |
| 1011 | conc<br>o170 | 3.320300E-07 | 3.094580E-07 | 2.257196E-08  | 1.000 |
| 1012 | conc<br>o171 | 3.354300E-07 | 3.025702E-07 | 3.285975E-08  | 1.000 |
| 1013 | conc<br>o172 | 3.396930E-07 | 2.952703E-07 | 4.442265E-08  | 1.000 |
| 1014 | conc<br>o173 | 3.431300E-07 | 2.876469E-07 | 5.548312E-08  | 1.000 |
| 1015 | conc<br>o174 | 3.395130E-07 | 2.797845E-07 | 5.972848E-08  | 1.000 |
| 1016 | conc<br>o175 | 3.262010E-07 | 2.717633E-07 | 5.443774E-08  | 1.000 |
| 1017 | conc<br>o176 | 3.068900E-07 | 2.636577E-07 | 4.323234E-08  | 1.000 |
| 1018 | conc<br>o177 | 2.857790E-07 | 2.555365E-07 | 3.024253E-08  | 1.000 |
| 1019 | conc<br>o178 | 2.668110E-07 | 2.474622E-07 | 1.934876E-08  | 1.000 |
| 1020 | conc<br>o179 | 2.517910E-07 | 2.394912E-07 | 1.229976E-08  | 1.000 |
| 1021 | conc<br>o180 | 2.414640E-07 | 2.316734E-07 | 9.790572E-09  | 1.000 |
| 1022 | conc<br>o181 | 2.365650E-07 | 2.240525E-07 | 1.251245E-08  | 1.000 |
| 1023 | conc<br>o182 | 2.363110E-07 | 2.166664E-07 | 1.964462E-08  | 1.000 |
| 1024 | conc<br>o183 | 2.362840E-07 | 2.095470E-07 | 2.673701E-08  | 1.000 |
| 1025 | conc<br>o184 | 2.315340E-07 | 2.027211E-07 | 2.881290E-08  | 1.000 |
| 1026 | conc<br>o185 | 2.175590E-07 | 1.962105E-07 | 2.134853E-08  | 1.000 |
| 1027 | conc<br>o186 | 1.970180E-07 | 1.900323E-07 | 6.985718E-09  | 1.000 |
| 1028 | conc<br>o187 | 1.783120E-07 | 1.841996E-07 | -5.887595E-09 | 1.000 |
| 1029 | conc<br>o188 | 1.700010E-07 | 1.787217E-07 | -8.720711E-09 | 1.000 |
| 1030 | conc<br>o189 | 1.777150E-07 | 1.736046E-07 | 4.110413E-09  | 1.000 |
| 1031 | conc<br>o190 | 1.951580E-07 | 1.688512E-07 | 2.630680E-08  | 1.000 |
| 1032 | conc<br>o191 | 2.130090E-07 | 1.644619E-07 | 4.854713E-08  | 1.000 |
| 1033 | conc<br>o192 | 2.220980E-07 | 1.604346E-07 | 6.166340E-08  | 1.000 |
| 1034 | conc<br>o193 | 2.190210E-07 | 1.567653E-07 | 6.225571E-08  | 1.000 |
| 1035 | conc<br>o194 | 2.077680E-07 | 1.534480E-07 | 5.431999E-08  | 1.000 |
| 1036 | conc<br>o195 | 1.928170E-07 | 1.504752E-07 | 4.234181E-08  | 1.000 |
| 1037 | conc<br>o196 | 1.781330E-07 | 1.478377E-07 | 3.029525E-08  | 1.000 |
| 1038 | conc<br>o197 | 1.640790E-07 | 1.455253E-07 | 1.855370E-08  | 1.000 |
| 1039 | conc<br>o198 | 1.494680E-07 | 1.435262E-07 | 5.941815E-09  | 1.000 |
| 1040 | conc<br>o199 | 1.331190E-07 | 1.418276E-07 | -8.708632E-09 | 1.000 |
| 1041 | conc<br>o200 | 1.157390E-07 | 1.404158E-07 | -2.467679E-08 | 1.000 |

|      |              |              |              |               |       |
|------|--------------|--------------|--------------|---------------|-------|
| 1042 | o201<br>conc | 1.019720E-07 | 1.392758E-07 | -3.730380E-08 | 1.000 |
| 1043 | o202<br>conc | 9.694750E-08 | 1.383919E-07 | -4.144437E-08 | 1.000 |
| 1044 | o203<br>conc | 1.051370E-07 | 1.377473E-07 | -3.261034E-08 | 1.000 |
| 1045 | o204<br>conc | 1.223640E-07 | 1.373247E-07 | -1.496068E-08 | 1.000 |
| 1046 | o205<br>conc | 1.383770E-07 | 1.371056E-07 | 1.271351E-09  | 1.000 |
| 1047 | o206<br>conc | 1.428050E-07 | 1.370713E-07 | 5.733719E-09  | 1.000 |
| 1048 | o207<br>conc | 1.314920E-07 | 1.372020E-07 | -5.710016E-09 | 1.000 |
| 1049 | o208<br>conc | 1.220170E-07 | 1.374778E-07 | -1.546077E-08 | 1.000 |
| 1050 | o209<br>conc | 1.310930E-07 | 1.378781E-07 | -6.785063E-09 | 1.000 |
| 1051 | o210<br>conc | 1.516410E-07 | 1.383821E-07 | 1.325891E-08  | 1.000 |
| 1052 | o211<br>conc | 1.702820E-07 | 1.389689E-07 | 3.131311E-08  | 1.000 |
| 1053 | o212<br>conc | 1.738790E-07 | 1.396175E-07 | 3.426154E-08  | 1.000 |
| 1054 | o213<br>conc | 1.592060E-07 | 1.403069E-07 | 1.889910E-08  | 1.000 |
| 1055 | o214<br>conc | 1.362240E-07 | 1.410166E-07 | -4.792569E-09 | 1.000 |
| 1056 | o215<br>conc | 1.158070E-07 | 1.417262E-07 | -2.591922E-08 | 1.000 |
| 1057 | o216<br>conc | 1.075060E-07 | 1.424162E-07 | -3.491019E-08 | 1.000 |
| 1058 | o217<br>conc | 1.111280E-07 | 1.430675E-07 | -3.193951E-08 | 1.000 |
| 1059 | o218<br>conc | 1.221220E-07 | 1.436621E-07 | -2.154009E-08 | 1.000 |
| 1060 | o219<br>conc | 1.359230E-07 | 1.441828E-07 | -8.259832E-09 | 1.000 |
| 1061 | o220<br>conc | 1.490340E-07 | 1.446138E-07 | 4.420214E-09  | 1.000 |
| 1062 | o221<br>conc | 1.602590E-07 | 1.449403E-07 | 1.531873E-08  | 1.000 |
| 1063 | o222<br>conc | 1.687090E-07 | 1.451490E-07 | 2.356005E-08  | 1.000 |
| 1064 | o223<br>conc | 1.735440E-07 | 1.452280E-07 | 2.831601E-08  | 1.000 |
| 1065 | o224<br>conc | 1.746890E-07 | 1.451671E-07 | 2.952194E-08  | 1.000 |
| 1066 | o225<br>conc | 1.726160E-07 | 1.449575E-07 | 2.765854E-08  | 1.000 |
| 1067 | o226<br>conc | 1.678140E-07 | 1.445921E-07 | 2.322190E-08  | 1.000 |
| 1068 | o227<br>conc | 1.609850E-07 | 1.440656E-07 | 1.691943E-08  | 1.000 |
| 1069 | o228<br>conc | 1.536160E-07 | 1.433741E-07 | 1.024189E-08  | 1.000 |
| 1070 | o229<br>conc | 1.473760E-07 | 1.425156E-07 | 4.860388E-09  | 1.000 |
| 1071 | o230<br>conc | 1.439010E-07 | 1.414896E-07 | 2.411428E-09  | 1.000 |
| 1072 | o231<br>conc | 1.439110E-07 | 1.402970E-07 | 3.613954E-09  | 1.000 |
| 1073 | o232<br>conc | 1.470550E-07 | 1.389406E-07 | 8.114422E-09  | 1.000 |
| 1074 | o233<br>conc | 1.529210E-07 | 1.374241E-07 | 1.549688E-08  | 1.000 |
| 1075 | o234<br>conc | 1.607910E-07 | 1.357529E-07 | 2.503807E-08  | 1.000 |
| 1076 | o235<br>conc | 1.680200E-07 | 1.339335E-07 | 3.408652E-08  | 1.000 |
| 1077 | o236<br>conc | 1.712170E-07 | 1.319733E-07 | 3.924367E-08  | 1.000 |
| 1078 | o237         | 1.670130E-07 | 1.298810E-07 | 3.713202E-08  | 1.000 |

|      |              |              |              |               |       |
|------|--------------|--------------|--------------|---------------|-------|
| 1079 | conc<br>o238 | 1.547170E-07 | 1.276658E-07 | 2.705118E-08  | 1.000 |
| 1080 | conc<br>o239 | 1.386780E-07 | 1.253379E-07 | 1.334011E-08  | 1.000 |
| 1081 | conc<br>o240 | 1.238020E-07 | 1.229079E-07 | 8.941448E-10  | 1.000 |
| 1082 | conc<br>o241 | 1.146300E-07 | 1.203868E-07 | -5.756787E-09 | 1.000 |
| 1083 | conc<br>o242 | 1.115150E-07 | 1.177861E-07 | -6.271087E-09 | 1.000 |
| 1084 | conc<br>o243 | 1.121430E-07 | 1.151173E-07 | -2.974340E-09 | 1.000 |
| 1085 | conc<br>o244 | 1.141600E-07 | 1.123922E-07 | 1.767803E-09  | 1.000 |
| 1086 | conc<br>o245 | 1.158380E-07 | 1.096223E-07 | 6.215737E-09  | 1.000 |
| 1087 | conc<br>o246 | 1.174180E-07 | 1.068190E-07 | 1.059902E-08  | 1.000 |
| 1088 | conc<br>o247 | 1.195250E-07 | 1.039936E-07 | 1.553145E-08  | 1.000 |
| 1089 | conc<br>o248 | 1.227500E-07 | 1.011568E-07 | 2.159318E-08  | 1.000 |
| 1090 | conc<br>o249 | 1.267810E-07 | 9.831922E-08 | 2.846178E-08  | 1.000 |
| 1091 | conc<br>o250 | 1.303900E-07 | 9.549069E-08 | 3.489931E-08  | 1.000 |
| 1092 | conc<br>o251 | 1.323070E-07 | 9.268059E-08 | 3.962641E-08  | 1.000 |
| 1093 | conc<br>o252 | 1.312620E-07 | 8.989772E-08 | 4.136428E-08  | 1.000 |
| 1094 | conc<br>o253 | 1.259960E-07 | 8.715022E-08 | 3.884578E-08  | 1.000 |
| 1095 | conc<br>o254 | 1.164210E-07 | 8.444553E-08 | 3.197547E-08  | 1.000 |
| 1096 | conc<br>o255 | 1.044990E-07 | 8.179043E-08 | 2.270857E-08  | 1.000 |
| 1097 | conc<br>o256 | 9.240340E-08 | 7.919098E-08 | 1.321242E-08  | 1.000 |
| 1098 | conc<br>o257 | 8.230520E-08 | 7.665254E-08 | 5.652663E-09  | 1.000 |
| 1099 | conc<br>o258 | 7.637660E-08 | 7.417974E-08 | 2.196861E-09  | 1.000 |
| 1100 | conc<br>o259 | 7.622740E-08 | 7.177653E-08 | 4.450867E-09  | 1.000 |
| 1101 | conc<br>o260 | 8.043840E-08 | 6.944619E-08 | 1.099221E-08  | 1.000 |
| 1102 | conc<br>o261 | 8.657490E-08 | 6.719132E-08 | 1.938358E-08  | 1.000 |
| 1103 | conc<br>o262 | 9.220160E-08 | 6.501390E-08 | 2.718770E-08  | 1.000 |
| 1104 | conc<br>o263 | 9.488300E-08 | 6.291532E-08 | 3.196768E-08  | 1.000 |
| 1105 | conc<br>o264 | 9.228590E-08 | 6.089639E-08 | 3.138951E-08  | 1.000 |
| 1106 | conc<br>o265 | 8.425190E-08 | 5.895741E-08 | 2.529449E-08  | 1.000 |
| 1107 | conc<br>o266 | 7.270670E-08 | 5.709818E-08 | 1.560852E-08  | 1.000 |
| 1108 | conc<br>o267 | 5.965960E-08 | 5.531804E-08 | 4.341557E-09  | 1.000 |
| 1109 | conc<br>o268 | 4.711980E-08 | 5.361596E-08 | -6.496162E-09 | 1.000 |
| 1110 | conc<br>o269 | 3.709570E-08 | 5.199052E-08 | -1.489482E-08 | 1.000 |
| 1111 | conc<br>o270 | 3.087830E-08 | 5.043998E-08 | -1.956168E-08 | 1.000 |
| 1112 | conc<br>o271 | 2.781440E-08 | 4.896231E-08 | -2.114791E-08 | 1.000 |
| 1113 | conc<br>o272 | 2.692480E-08 | 4.755527E-08 | -2.063047E-08 | 1.000 |
| 1114 | conc<br>o273 | 2.723000E-08 | 4.621638E-08 | -1.898638E-08 | 1.000 |

|      |              |              |              |               |       |
|------|--------------|--------------|--------------|---------------|-------|
| 1115 | o274<br>conc | 2.775070E-08 | 4.494301E-08 | -1.719231E-08 | 1.000 |
| 1116 | o275<br>conc | 2.760460E-08 | 4.373240E-08 | -1.612780E-08 | 1.000 |
| 1117 | o276<br>conc | 2.676470E-08 | 4.258169E-08 | -1.581699E-08 | 1.000 |
| 1118 | o277<br>conc | 2.564830E-08 | 4.148794E-08 | -1.583964E-08 | 1.000 |
| 1119 | o278<br>conc | 2.467640E-08 | 4.044818E-08 | -1.577178E-08 | 1.000 |
| 1120 | o279<br>conc | 2.427000E-08 | 3.945944E-08 | -1.518944E-08 | 1.000 |
| 1121 | o280<br>conc | 2.484250E-08 | 3.851874E-08 | -1.367624E-08 | 1.000 |
| 1122 | o281<br>conc | 2.641960E-08 | 3.762314E-08 | -1.120354E-08 | 1.000 |
| 1123 | o282<br>conc | 2.847000E-08 | 3.676975E-08 | -8.299752E-09 | 1.000 |
| 1124 | o283<br>conc | 3.041950E-08 | 3.595576E-08 | -5.536257E-09 | 1.000 |
| 1125 | o284<br>conc | 3.169390E-08 | 3.517842E-08 | -3.484517E-09 | 1.000 |
| 1126 | o285<br>conc | 3.171880E-08 | 3.443509E-08 | -2.716291E-09 | 1.000 |
| 1127 | o286<br>conc | 3.013650E-08 | 3.372324E-08 | -3.586742E-09 | 1.000 |
| 1128 | o287<br>conc | 2.751750E-08 | 3.304045E-08 | -5.522948E-09 | 1.000 |
| 1129 | o288<br>conc | 2.468130E-08 | 3.238441E-08 | -7.703109E-09 | 1.000 |
| 1130 | o289<br>conc | 2.244710E-08 | 3.175295E-08 | -9.305850E-09 | 1.000 |
| 1131 | o290<br>conc | 2.163440E-08 | 3.114402E-08 | -9.509624E-09 | 1.000 |
| 1132 | o291<br>conc | 2.300960E-08 | 3.055572E-08 | -7.546116E-09 | 1.000 |
| 1133 | o292<br>conc | 2.652400E-08 | 2.998624E-08 | -3.462243E-09 | 1.000 |
| 1134 | o293<br>conc | 3.148730E-08 | 2.943395E-08 | 2.053346E-09  | 1.000 |
| 1135 | o294<br>conc | 3.719240E-08 | 2.889732E-08 | 8.295076E-09  | 1.000 |
| 1136 | o295<br>conc | 4.293170E-08 | 2.837496E-08 | 1.455674E-08  | 1.000 |
| 1137 | o296<br>conc | 4.799810E-08 | 2.786559E-08 | 2.013251E-08  | 1.000 |
| 1138 | o297<br>conc | 5.168400E-08 | 2.736806E-08 | 2.431594E-08  | 1.000 |
| 1139 | o298<br>conc | 5.328230E-08 | 2.688133E-08 | 2.640097E-08  | 1.000 |
| 1140 | o299<br>conc | 5.226800E-08 | 2.640447E-08 | 2.586353E-08  | 1.000 |
| 1141 | o300<br>conc | 4.918680E-08 | 2.593667E-08 | 2.325013E-08  | 1.000 |
| 1142 | o301<br>conc | 4.497330E-08 | 2.547719E-08 | 1.949611E-08  | 1.000 |
| 1143 | o302<br>conc | 4.056260E-08 | 2.502540E-08 | 1.553720E-08  | 1.000 |
| 1144 | o303<br>conc | 3.689010E-08 | 2.458076E-08 | 1.230934E-08  | 1.000 |
| 1145 | o304<br>conc | 3.486190E-08 | 2.414280E-08 | 1.071910E-08  | 1.000 |
| 1146 | o305<br>conc | 3.468440E-08 | 2.371112E-08 | 1.097328E-08  | 1.000 |
| 1147 | o306<br>conc | 3.584280E-08 | 2.328540E-08 | 1.255740E-08  | 1.000 |
| 1148 | o307<br>conc | 3.778920E-08 | 2.286537E-08 | 1.492383E-08  | 1.000 |
| 1149 | o308<br>conc | 3.997600E-08 | 2.245083E-08 | 1.752517E-08  | 1.000 |
| 1150 | o309<br>conc | 4.185520E-08 | 2.204161E-08 | 1.981359E-08  | 1.000 |
| 1151 | o310         | 4.287920E-08 | 2.163760E-08 | 2.124160E-08  | 1.000 |

|      |              |              |              |              |       |
|------|--------------|--------------|--------------|--------------|-------|
| 1152 | conc<br>o311 | 4.250540E-08 | 2.123872E-08 | 2.126668E-08 | 1.000 |
| 1153 | conc<br>o312 | 4.056860E-08 | 2.084492E-08 | 1.972368E-08 | 1.000 |
| 1154 | conc<br>o313 | 3.752820E-08 | 2.045620E-08 | 1.707200E-08 | 1.000 |
| 1155 | conc<br>o314 | 3.390200E-08 | 2.007256E-08 | 1.382944E-08 | 1.000 |
| 1156 | conc<br>o315 | 3.020810E-08 | 1.969404E-08 | 1.051406E-08 | 1.000 |
| 1157 | conc<br>o316 | 2.696450E-08 | 1.932066E-08 | 7.643837E-09 | 1.000 |
| 1158 | conc<br>o317 | 2.468900E-08 | 1.895251E-08 | 5.736494E-09 | 1.000 |
| 1159 | conc<br>o318 | 2.389950E-08 | 1.858963E-08 | 5.309871E-09 | 1.000 |
| 1160 | conc<br>o319 | 2.486570E-08 | 1.823211E-08 | 6.633593E-09 | 1.000 |
| 1161 | conc<br>o320 | 2.718140E-08 | 1.788002E-08 | 9.301384E-09 | 1.000 |
| 1162 | conc<br>o321 | 3.032590E-08 | 1.753343E-08 | 1.279247E-08 | 1.000 |
| 1163 | conc<br>o322 | 3.377870E-08 | 1.719244E-08 | 1.658626E-08 | 1.000 |
| 1164 | conc<br>o323 | 3.701890E-08 | 1.685711E-08 | 2.016179E-08 | 1.000 |
| 1165 | conc<br>o324 | 3.952600E-08 | 1.652750E-08 | 2.299850E-08 | 1.000 |
| 1166 | conc<br>o325 | 4.077930E-08 | 1.620369E-08 | 2.457561E-08 | 1.000 |
| 1167 | conc<br>o326 | 4.038680E-08 | 1.588573E-08 | 2.450107E-08 | 1.000 |
| 1168 | conc<br>o327 | 3.855690E-08 | 1.557367E-08 | 2.298323E-08 | 1.000 |
| 1169 | conc<br>o328 | 3.567240E-08 | 1.526755E-08 | 2.040485E-08 | 1.000 |
| 1170 | conc<br>o329 | 3.211630E-08 | 1.496739E-08 | 1.714891E-08 | 1.000 |
| 1171 | conc<br>o330 | 2.827140E-08 | 1.467323E-08 | 1.359817E-08 | 1.000 |
| 1172 | conc<br>o331 | 2.452070E-08 | 1.438507E-08 | 1.013563E-08 | 1.000 |
| 1173 | conc<br>o332 | 2.124710E-08 | 1.410291E-08 | 7.144189E-09 | 1.000 |
| 1174 | conc<br>o333 | 1.879250E-08 | 1.382675E-08 | 4.965754E-09 | 1.000 |
| 1175 | conc<br>o334 | 1.716460E-08 | 1.355656E-08 | 3.608044E-09 | 1.000 |
| 1176 | conc<br>o335 | 1.620760E-08 | 1.329231E-08 | 2.915288E-09 | 1.000 |
| 1177 | conc<br>o336 | 1.576470E-08 | 1.303398E-08 | 2.730723E-09 | 1.000 |
| 1178 | conc<br>o337 | 1.567900E-08 | 1.278150E-08 | 2.897496E-09 | 1.000 |
| 1179 | conc<br>o338 | 1.579370E-08 | 1.253484E-08 | 3.258862E-09 | 1.000 |
| 1180 | conc<br>o339 | 1.595200E-08 | 1.229391E-08 | 3.658085E-09 | 1.000 |
| 1181 | conc<br>o340 | 1.600030E-08 | 1.205866E-08 | 3.941636E-09 | 1.000 |
| 1182 | conc<br>o341 | 1.587080E-08 | 1.182901E-08 | 4.041792E-09 | 1.000 |
| 1183 | conc<br>o342 | 1.558860E-08 | 1.160486E-08 | 3.983738E-09 | 1.000 |
| 1184 | conc<br>o343 | 1.518340E-08 | 1.138614E-08 | 3.797264E-09 | 1.000 |
| 1185 | conc<br>o344 | 1.468500E-08 | 1.117274E-08 | 3.512265E-09 | 1.000 |
| 1186 | conc<br>o345 | 1.412300E-08 | 1.096456E-08 | 3.158441E-09 | 1.000 |
| 1187 | conc<br>o346 | 1.352730E-08 | 1.076150E-08 | 2.765796E-09 | 1.000 |

|      |              |              |              |              |       |
|------|--------------|--------------|--------------|--------------|-------|
| 1188 | o347<br>conc | 1.292740E-08 | 1.056346E-08 | 2.363937E-09 | 1.000 |
| 1189 | o348<br>conc | 1.234810E-08 | 1.037032E-08 | 1.977776E-09 | 1.000 |
| 1190 | o349<br>conc | 1.180590E-08 | 1.018198E-08 | 1.623925E-09 | 1.000 |
| 1191 | o350<br>conc | 1.131620E-08 | 9.998302E-09 | 1.317898E-09 | 1.000 |
| 1192 | o351<br>conc | 1.089450E-08 | 9.819187E-09 | 1.075313E-09 | 1.000 |
| 1193 | o352<br>conc | 1.055630E-08 | 9.644515E-09 | 9.117851E-10 | 1.000 |
| 1194 | o353<br>conc | 1.031710E-08 | 9.474167E-09 | 8.429331E-10 | 1.000 |
| 1195 | o354<br>conc | 1.019230E-08 | 9.308026E-09 | 8.842742E-10 | 1.000 |
| 1196 | o355<br>conc | 1.018390E-08 | 9.145974E-09 | 1.037926E-09 | 1.000 |
| 1197 | o356<br>conc | 1.025410E-08 | 8.987895E-09 | 1.266205E-09 | 1.000 |
| 1198 | o357<br>conc | 1.035830E-08 | 8.833674E-09 | 1.524626E-09 | 1.000 |
| 1199 | o358<br>conc | 1.045180E-08 | 8.683195E-09 | 1.768605E-09 | 1.000 |
| 1200 | o359<br>conc | 1.048990E-08 | 8.536346E-09 | 1.953554E-09 | 1.000 |
| 1201 | o360<br>conc | 1.042780E-08 | 8.393016E-09 | 2.034784E-09 | 1.000 |
| 1202 | o361<br>conc | 1.022100E-08 | 8.253095E-09 | 1.967905E-09 | 1.000 |
| 1203 | o362<br>conc | 9.846240E-09 | 8.116478E-09 | 1.729762E-09 | 1.000 |
| 1204 | o363<br>conc | 9.387050E-09 | 7.983058E-09 | 1.403992E-09 | 1.000 |
| 1205 | o364<br>conc | 8.959660E-09 | 7.852735E-09 | 1.106925E-09 | 1.000 |
| 1206 | o365<br>conc | 8.680350E-09 | 7.725408E-09 | 9.549417E-10 | 1.000 |
| 1207 | o366<br>conc | 8.665390E-09 | 7.600981E-09 | 1.064409E-09 | 1.000 |
| 1208 | o367<br>conc | 9.031040E-09 | 7.479360E-09 | 1.551680E-09 | 1.000 |
| 1209 | o368<br>conc | 9.893570E-09 | 7.360453E-09 | 2.533117E-09 | 1.000 |
| 1210 | o369<br>conc | 1.134860E-08 | 7.244172E-09 | 4.104428E-09 | 1.000 |
| 1211 | o370<br>conc | 1.331210E-08 | 7.130430E-09 | 6.181670E-09 | 1.000 |
| 1212 | o371<br>conc | 1.560750E-08 | 7.019147E-09 | 8.588353E-09 | 1.000 |
| 1213 | o372<br>conc | 1.805770E-08 | 6.910240E-09 | 1.114746E-08 | 1.000 |
| 1214 | o373<br>conc | 2.048540E-08 | 6.803634E-09 | 1.368177E-08 | 1.000 |
| 1215 | o374<br>conc | 2.271350E-08 | 6.699253E-09 | 1.601425E-08 | 1.000 |
| 1216 | o375<br>conc | 2.456470E-08 | 6.597027E-09 | 1.796767E-08 | 1.000 |
| 1217 | o376<br>conc | 2.587030E-08 | 6.496887E-09 | 1.937341E-08 | 1.000 |
| 1218 | o377<br>conc | 2.660560E-08 | 6.398765E-09 | 2.020683E-08 | 1.000 |
| 1219 | o378<br>conc | 2.686570E-08 | 6.302599E-09 | 2.056310E-08 | 1.000 |
| 1220 | o379<br>conc | 2.674930E-08 | 6.208328E-09 | 2.054097E-08 | 1.000 |
| 1221 | o380<br>conc | 2.635510E-08 | 6.115893E-09 | 2.023921E-08 | 1.000 |
| 1222 | o381<br>conc | 2.578180E-08 | 6.025237E-09 | 1.975656E-08 | 1.000 |
| 1223 | o382<br>conc | 2.512810E-08 | 5.936307E-09 | 1.919179E-08 | 1.000 |
| 1224 | o383         | 2.448710E-08 | 5.849051E-09 | 1.863805E-08 | 1.000 |

|      |              |              |              |              |       |
|------|--------------|--------------|--------------|--------------|-------|
| 1225 | conc<br>o384 | 2.393560E-08 | 5.763419E-09 | 1.817218E-08 | 1.000 |
| 1226 | conc<br>o385 | 2.354760E-08 | 5.679365E-09 | 1.786824E-08 | 1.000 |
| 1227 | conc<br>o386 | 2.339700E-08 | 5.596842E-09 | 1.780016E-08 | 1.000 |
| 1228 | conc<br>o387 | 2.355770E-08 | 5.515807E-09 | 1.804189E-08 | 1.000 |
| 1229 | conc<br>o388 | 2.410370E-08 | 5.436218E-09 | 1.866748E-08 | 1.000 |
| 1230 | conc<br>o389 | 2.510890E-08 | 5.358036E-09 | 1.975086E-08 | 1.000 |
| 1231 | conc<br>o390 | 2.660560E-08 | 5.281222E-09 | 2.132438E-08 | 1.000 |
| 1232 | conc<br>o391 | 2.841940E-08 | 5.205739E-09 | 2.321366E-08 | 1.000 |
| 1233 | conc<br>o392 | 3.031210E-08 | 5.131553E-09 | 2.518055E-08 | 1.000 |
| 1234 | conc<br>o393 | 3.204560E-08 | 5.058629E-09 | 2.698697E-08 | 1.000 |
| 1235 | conc<br>o394 | 3.338170E-08 | 4.986935E-09 | 2.839476E-08 | 1.000 |
| 1236 | conc<br>o395 | 3.408220E-08 | 4.916441E-09 | 2.916576E-08 | 1.000 |
| 1237 | conc<br>o396 | 3.390880E-08 | 4.847117E-09 | 2.906168E-08 | 1.000 |
| 1238 | conc<br>o397 | 3.266310E-08 | 4.778934E-09 | 2.788417E-08 | 1.000 |
| 1239 | conc<br>o398 | 3.049240E-08 | 4.711865E-09 | 2.578054E-08 | 1.000 |
| 1240 | conc<br>o399 | 2.772300E-08 | 4.645883E-09 | 2.307712E-08 | 1.000 |
| 1241 | conc<br>o400 | 2.468260E-08 | 4.580964E-09 | 2.010164E-08 | 1.000 |
| 1242 | conc<br>o401 | 2.169880E-08 | 4.517084E-09 | 1.718172E-08 | 1.000 |
| 1243 | conc<br>o402 | 1.909940E-08 | 4.454218E-09 | 1.464518E-08 | 1.000 |
| 1244 | conc<br>o403 | 1.721200E-08 | 4.392344E-09 | 1.281966E-08 | 1.000 |
| 1245 | conc<br>o404 | 1.634920E-08 | 4.331442E-09 | 1.201776E-08 | 1.000 |
| 1246 | conc<br>o405 | 1.656890E-08 | 4.271489E-09 | 1.229741E-08 | 1.000 |
| 1247 | conc<br>o406 | 1.771620E-08 | 4.212466E-09 | 1.350373E-08 | 1.000 |
| 1248 | conc<br>o407 | 1.962940E-08 | 4.154354E-09 | 1.547505E-08 | 1.000 |
| 1249 | conc<br>o408 | 2.214720E-08 | 4.097133E-09 | 1.805007E-08 | 1.000 |
| 1250 | conc<br>o409 | 2.510800E-08 | 4.040787E-09 | 2.106721E-08 | 1.000 |
| 1251 | conc<br>o410 | 2.835030E-08 | 3.985296E-09 | 2.436500E-08 | 1.000 |
| 1252 | conc<br>o411 | 3.171240E-08 | 3.930645E-09 | 2.778176E-08 | 1.000 |
| 1253 | conc<br>o412 | 3.502540E-08 | 3.876816E-09 | 3.114858E-08 | 1.000 |
| 1254 | conc<br>o413 | 3.811070E-08 | 3.823795E-09 | 3.428691E-08 | 1.000 |
| 1255 | conc<br>o414 | 4.078870E-08 | 3.771565E-09 | 3.701713E-08 | 1.000 |
| 1256 | conc<br>o415 | 4.288030E-08 | 3.720113E-09 | 3.916019E-08 | 1.000 |
| 1257 | conc<br>o416 | 4.420600E-08 | 3.669423E-09 | 4.053658E-08 | 1.000 |
| 1258 | conc<br>o417 | 4.458640E-08 | 3.619481E-09 | 4.096692E-08 | 1.000 |
| 1259 | conc<br>o418 | 4.384330E-08 | 3.570274E-09 | 4.027303E-08 | 1.000 |
| 1260 | conc<br>o419 | 4.198300E-08 | 3.521788E-09 | 3.846121E-08 | 1.000 |

|      |              |              |              |              |       |
|------|--------------|--------------|--------------|--------------|-------|
| 1261 | o420<br>conc | 3.941400E-08 | 3.474012E-09 | 3.593999E-08 | 1.000 |
| 1262 | o421<br>conc | 3.659730E-08 | 3.426931E-09 | 3.317037E-08 | 1.000 |
| 1263 | o422<br>conc | 3.399400E-08 | 3.380534E-09 | 3.061347E-08 | 1.000 |
| 1264 | o423<br>conc | 3.204760E-08 | 3.334810E-09 | 2.871279E-08 | 1.000 |
| 1265 | o424<br>conc | 3.086660E-08 | 3.289745E-09 | 2.757685E-08 | 1.000 |
| 1266 | o425<br>conc | 3.025930E-08 | 3.245330E-09 | 2.701397E-08 | 1.000 |
| 1267 | o426<br>conc | 3.002380E-08 | 3.201553E-09 | 2.682225E-08 | 1.000 |
| 1268 | o427<br>conc | 2.995800E-08 | 3.158404E-09 | 2.679960E-08 | 1.000 |
| 1269 | o428<br>conc | 2.985980E-08 | 3.115871E-09 | 2.674393E-08 | 1.000 |
| 1270 | o429<br>conc | 2.952710E-08 | 3.073945E-09 | 2.645315E-08 | 1.000 |
| 1271 | o430<br>conc | 2.876140E-08 | 3.032616E-09 | 2.572878E-08 | 1.000 |
| 1272 | o431<br>conc | 2.753560E-08 | 2.991873E-09 | 2.454373E-08 | 1.000 |
| 1273 | o432<br>conc | 2.606870E-08 | 2.951708E-09 | 2.311699E-08 | 1.000 |
| 1274 | o433<br>conc | 2.459860E-08 | 2.912111E-09 | 2.168649E-08 | 1.000 |
| 1275 | o434<br>conc | 2.336330E-08 | 2.873072E-09 | 2.049023E-08 | 1.000 |
| 1276 | o435<br>conc | 2.260070E-08 | 2.834584E-09 | 1.976612E-08 | 1.000 |
| 1277 | o436<br>conc | 2.254880E-08 | 2.796636E-09 | 1.975216E-08 | 1.000 |
| 1278 | o437<br>conc | 2.344480E-08 | 2.759221E-09 | 2.068558E-08 | 1.000 |
| 1279 | o438<br>conc | 2.536450E-08 | 2.722330E-09 | 2.264217E-08 | 1.000 |
| 1280 | o439<br>conc | 2.800460E-08 | 2.685954E-09 | 2.531865E-08 | 1.000 |
| 1281 | o440<br>conc | 3.100760E-08 | 2.650087E-09 | 2.835751E-08 | 1.000 |
| 1282 | o441<br>conc | 3.401610E-08 | 2.614719E-09 | 3.140138E-08 | 1.000 |
| 1283 | o442<br>conc | 3.667270E-08 | 2.579843E-09 | 3.409286E-08 | 1.000 |
| 1284 | o443<br>conc | 3.862000E-08 | 2.545452E-09 | 3.607455E-08 | 1.000 |
| 1285 | o444<br>conc | 3.950070E-08 | 2.511538E-09 | 3.698916E-08 | 1.000 |
| 1286 | o445<br>conc | 3.908620E-08 | 2.478093E-09 | 3.660811E-08 | 1.000 |
| 1287 | o446<br>conc | 3.766020E-08 | 2.445111E-09 | 3.521509E-08 | 1.000 |
| 1288 | o447<br>conc | 3.563300E-08 | 2.412584E-09 | 3.322042E-08 | 1.000 |
| 1289 | o448<br>conc | 3.341490E-08 | 2.380506E-09 | 3.103439E-08 | 1.000 |
| 1290 | o449<br>conc | 3.141630E-08 | 2.348869E-09 | 2.906743E-08 | 1.000 |
| 1291 | o450<br>conc | 3.004740E-08 | 2.317668E-09 | 2.772973E-08 | 1.000 |
| 1292 | o451<br>conc | 2.971880E-08 | 2.286895E-09 | 2.743191E-08 | 1.000 |
| 1293 | o452<br>conc | 3.075270E-08 | 2.256544E-09 | 2.849616E-08 | 1.000 |
| 1294 | o453<br>conc | 3.286720E-08 | 2.226609E-09 | 3.064059E-08 | 1.000 |
| 1295 | o454<br>conc | 3.552650E-08 | 2.197084E-09 | 3.332942E-08 | 1.000 |
| 1296 | o455<br>conc | 3.819390E-08 | 2.167962E-09 | 3.602594E-08 | 1.000 |
| 1297 | o456         | 4.033280E-08 | 2.139238E-09 | 3.819356E-08 | 1.000 |



|      |              |              |              |               |       |
|------|--------------|--------------|--------------|---------------|-------|
| 1298 | conc<br>o457 | 4.140650E-08 | 2.110905E-09 | 3.929559E-08  | 1.000 |
| 1299 | conc<br>o458 | 4.087830E-08 | 2.082958E-09 | 3.879534E-08  | 1.000 |
| 1300 | conc<br>o459 | 3.826280E-08 | 2.055392E-09 | 3.620741E-08  | 1.000 |
| 1301 | conc<br>o460 | 3.372330E-08 | 2.028200E-09 | 3.169510E-08  | 1.000 |
| 1302 | conc<br>o461 | 2.786850E-08 | 2.001377E-09 | 2.586712E-08  | 1.000 |
| 1303 | conc<br>o462 | 2.131620E-08 | 1.974919E-09 | 1.934128E-08  | 1.000 |
| 1304 | conc<br>o463 | 1.468380E-08 | 1.948818E-09 | 1.273498E-08  | 1.000 |
| 1305 | conc<br>o464 | 8.588990E-09 | 1.923071E-09 | 6.665919E-09  | 1.000 |
| 1306 | conc<br>o465 | 3.649360E-09 | 1.897672E-09 | 1.751688E-09  | 1.000 |
| 1307 | conc<br>o466 | 4.677260E-10 | 1.872616E-09 | -1.404890E-09 | 1.000 |
| 1308 | conc<br>o467 | 0.00000      | 1.847899E-09 | -1.847899E-09 | 1.000 |
| 1309 | conc<br>o468 | 0.00000      | 1.823515E-09 | -1.823515E-09 | 1.000 |
| 1310 | conc<br>o469 | 1.626740E-09 | 1.799459E-09 | -1.727189E-10 | 1.000 |
| 1311 | conc<br>o470 | 4.693200E-09 | 1.775727E-09 | 2.917473E-09  | 1.000 |
| 1312 | conc<br>o471 | 8.644330E-09 | 1.752314E-09 | 6.892016E-09  | 1.000 |
| 1313 | conc<br>o472 | 1.320690E-08 | 1.729216E-09 | 1.147768E-08  | 1.000 |
| 1314 | conc<br>o473 | 1.810750E-08 | 1.706429E-09 | 1.640107E-08  | 1.000 |
| 1315 | conc<br>o474 | 2.306840E-08 | 1.683947E-09 | 2.138445E-08  | 1.000 |
| 1316 | conc<br>o475 | 2.780330E-08 | 1.661766E-09 | 2.614153E-08  | 1.000 |
| 1317 | conc<br>o476 | 3.202510E-08 | 1.639883E-09 | 3.038522E-08  | 1.000 |
| 1318 | conc<br>o477 | 3.544690E-08 | 1.618292E-09 | 3.382861E-08  | 1.000 |
| 1319 | conc<br>o478 | 3.778170E-08 | 1.596990E-09 | 3.618471E-08  | 1.000 |
| 1320 | conc<br>o479 | 3.874230E-08 | 1.575974E-09 | 3.716633E-08  | 1.000 |
| 1321 | conc<br>o480 | 3.804200E-08 | 1.555237E-09 | 3.648676E-08  | 1.000 |
| 1322 | conc<br>o481 | 3.556310E-08 | 1.534778E-09 | 3.402832E-08  | 1.000 |
| 1323 | conc<br>o482 | 3.168540E-08 | 1.514592E-09 | 3.017081E-08  | 1.000 |
| 1324 | conc<br>o483 | 2.688000E-08 | 1.494675E-09 | 2.538533E-08  | 1.000 |
| 1325 | conc<br>o484 | 2.161760E-08 | 1.475023E-09 | 2.014258E-08  | 1.000 |
| 1326 | conc<br>o485 | 1.636920E-08 | 1.455633E-09 | 1.491357E-08  | 1.000 |
| 1327 | conc<br>o486 | 1.160560E-08 | 1.436500E-09 | 1.016910E-08  | 1.000 |
| 1328 | conc<br>o487 | 7.797780E-09 | 1.417623E-09 | 6.380157E-09  | 1.000 |
| 1329 | conc<br>o488 | 5.321320E-09 | 1.398996E-09 | 3.922324E-09  | 1.000 |
| 1330 | conc<br>o489 | 4.072160E-09 | 1.380617E-09 | 2.691543E-09  | 1.000 |
| 1331 | conc<br>o490 | 3.795720E-09 | 1.362481E-09 | 2.433239E-09  | 1.000 |
| 1332 | conc<br>o491 | 4.237380E-09 | 1.344587E-09 | 2.892793E-09  | 1.000 |
| 1333 | conc<br>o492 | 5.142490E-09 | 1.326929E-09 | 3.815561E-09  | 1.000 |

|      |      |              |              |              |       |
|------|------|--------------|--------------|--------------|-------|
| 1334 | o493 | 6.256440E-09 | 1.309506E-09 | 4.946934E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1335 | o494 | 7.324600E-09 | 1.292314E-09 | 6.032286E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1336 | o495 | 8.113290E-09 | 1.275349E-09 | 6.837941E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1337 | o496 | 8.575080E-09 | 1.258609E-09 | 7.316471E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1338 | o497 | 8.760030E-09 | 1.242090E-09 | 7.517940E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1339 | o498 | 8.719080E-09 | 1.225790E-09 | 7.493290E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1340 | o499 | 8.503150E-09 | 1.209705E-09 | 7.293445E-09 | 1.000 |
|      | conc |              |              |              |       |
| 1341 | o500 | 8.163170E-09 | 1.193833E-09 | 6.969337E-09 | 1.000 |
|      | conc |              |              |              |       |

1342  
1343 See file mfit.res for more details of residuals in graph-ready format.

1344  
1345 See file mfit.seo for composite observation sensitivities.

1346  
1347  
1348 Objective function ----->

1349 Sum of squared weighted residuals (ie phi) = 1.9587E-13

1351  
1352  
1353 Correlation Coefficient ----->

1354 Correlation coefficient = 0.98041

1356  
1357  
1358 Analysis of residuals ----->

1359 All residuals:-

|      |  |   |             |
|------|--|---|-------------|
| 1361 | Number of residuals with non-zero weight       | = | 447         |
| 1362 | Mean value of non-zero weighted residuals      | = | 1.2032E-08  |
| 1363 | Maximum weighted residual [observation "o193"] | = | 6.2256E-08  |
| 1364 | Minimum weighted residual [observation "o202"] | = | -4.1444E-08 |
| 1365 | Standard variance of weighted residuals        | = | 4.5029E-16  |
| 1366 | Standard error of weighted residuals           | = | 2.1220E-08  |

1367  
1368 Note: the above variance was obtained by dividing the objective  
1369 function by the number of system degrees of freedom (ie. number of  
1370 observations with non-zero weight plus number of prior information  
1371 articles with non-zero weight minus the number of adjustable parameters.)  
1372 If the degrees of freedom is negative the divisor becomes  
1373 the number of observations with non-zero weight plus the number of  
1374 prior information items with non-zero weight.

1375  
1376  
1377 Covariance and other statistical matrices cannot be determined:-  
1378 Memory conservation is operative so that covariance matrix is not calculated.

1379  
1380