given name of theory

any comment
short description

what to cite

theory (fit) parameters
! comment

parameter from
records

this is returned
as theory value

any specific
subroutines
and
functions to
be called in
the main
implementation

```
001   #THEORY locrep
002         generalized local reptation expression
003         along the lines of deGennes, but with finite summation of integrals
004         and lenthscale, timescale and fluctuation ratio as parameters
005   #CITE   P.G. De Gennes. Coherent scattering by one reptating chain.
006         Journal de Physique, 1981, 42 (5), pp.735-740. <10.1051/jphys:01981004205073500>
007   #PARAMETERS
008         ampli              ! prefactor
009         b                  ! fluctuation intensity (relative)
010         a                  ! length scale
011         tau                ! timescale
012         lz                 ! total length
013   #RECIN-PARAMETERS     (allow 8 chars for name, start only beyond 8 with default)
014         q            0   ! q-value    default value
015   #RECOUT-PARAMETERS
016   #VARIABLES
017       double precision   :: t
018   #IMPLEMENTATION
019       t = x                 ! since we prefer to call the independent variable t, x must be copied to t
020       th = ampli * local_reptation(q*a, t/tau, lz)
021
022   #SUBROUTINES
023     function local_reptation(q, t, L) result(val)
024       implicit none
025       double precision, intent(in)   :: q, t, L
026       double precision               :: val
027       double precision, parameter    :: sqp = sqrt(4*atan(1d0))
028
029       val = 0.72D2 * (sqrt(t) * q ** 4 * exp((-0.2D1 * L * q ** 2 * t -
030      #0.3D1 * L ** 2) / t / 0.12D2) / 0.36D2 + sqrt(0.3141592653589793D1
031      #) * (q ** 2 * t / 0.3D1 + L) * q ** 4 * exp(t * q ** 4 / 0.36D2) *
032      # (-erfc((q ** 2 * t + 0.3D1 * L) * t ** (-0.1D1 / 0.2D1) / 0.6D1)
033      #+ erfc(sqrt(t) * q ** 2 / 0.6D1)) / 0.72D2 - sqrt(t) * q ** 4 / 0.
034      #36D2) * B / q ** 4 * 0.3141592653589793D1 ** (-0.1D1 / 0.2D1) / L
035      #+ 0.72D2 * (A * exp(-q ** 2 * L / 0.6D1) * sqrt(0.3141592653589793
036      #D1) + (A * L * q ** 2 / 0.6D1 - A) * sqrt(0.3141592653589793D1)) *
037      # 0.3141592653589793D1 ** (-0.1D1 / 0.2D1) / q ** 4 / L
038
039
040     end function local_reptation
041   #END
```