

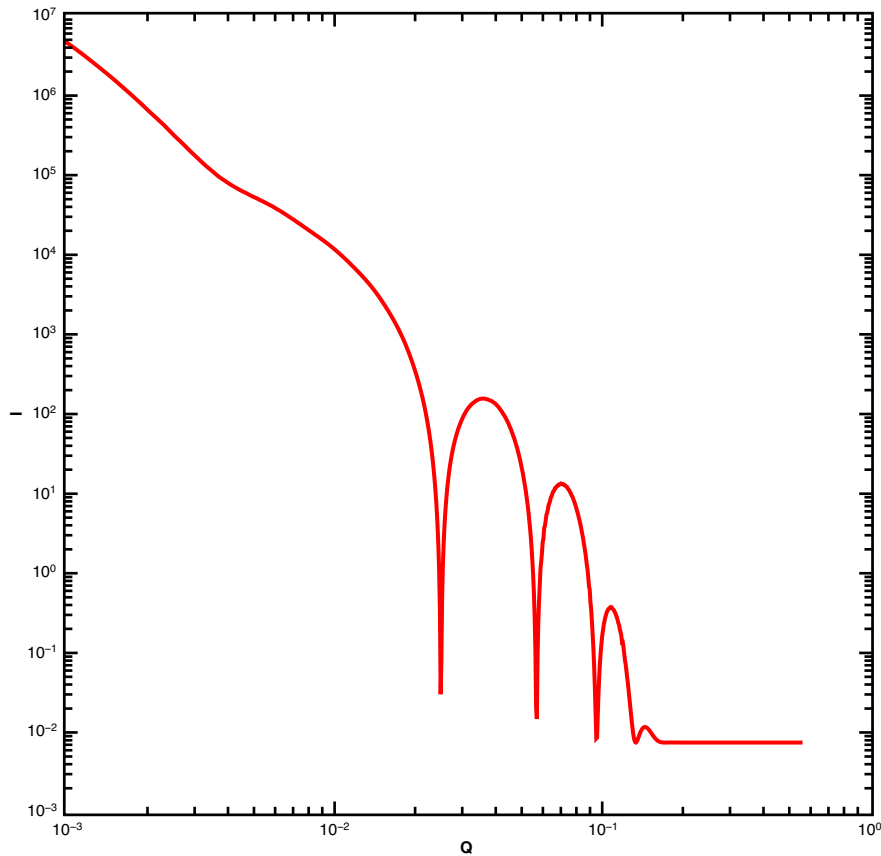


QtiSAS v. >2020

Using Fortran functions in Fit

# Using Fortran code in Fitting Functions

Multilamellar vesicle model



## Multilamellar Vesicle Model

Model author: Henrich Frielinghaus

Fortran code author: Henrich Frielinghaus

QtiKWS/QtiSAS integration: Vitaliy Pipich

Reference:

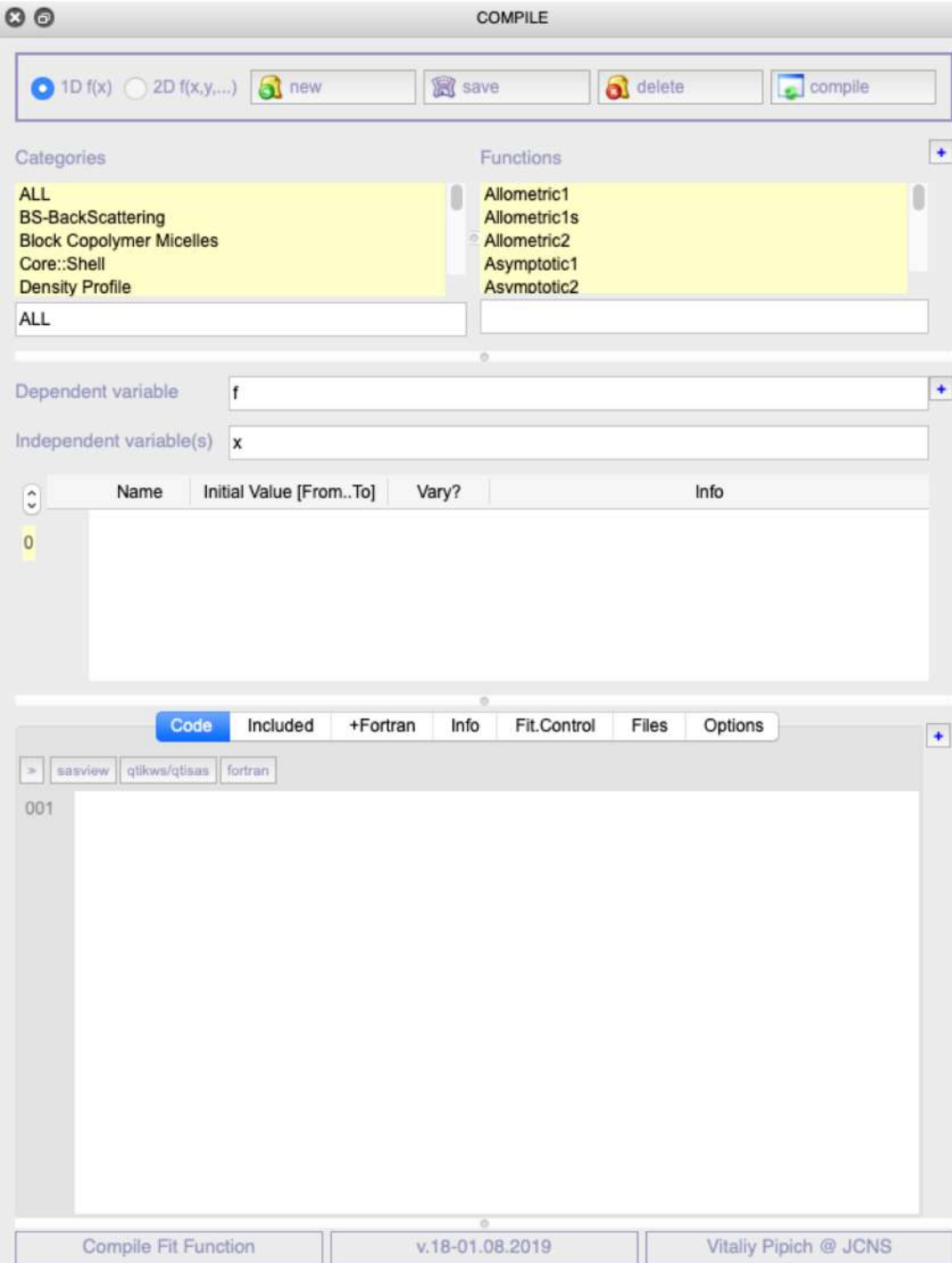
<https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603>

Fortran code: fortran-sphere-vesicle-mlv.f  
[move to "FitFunctions/IncludedFunctions"]

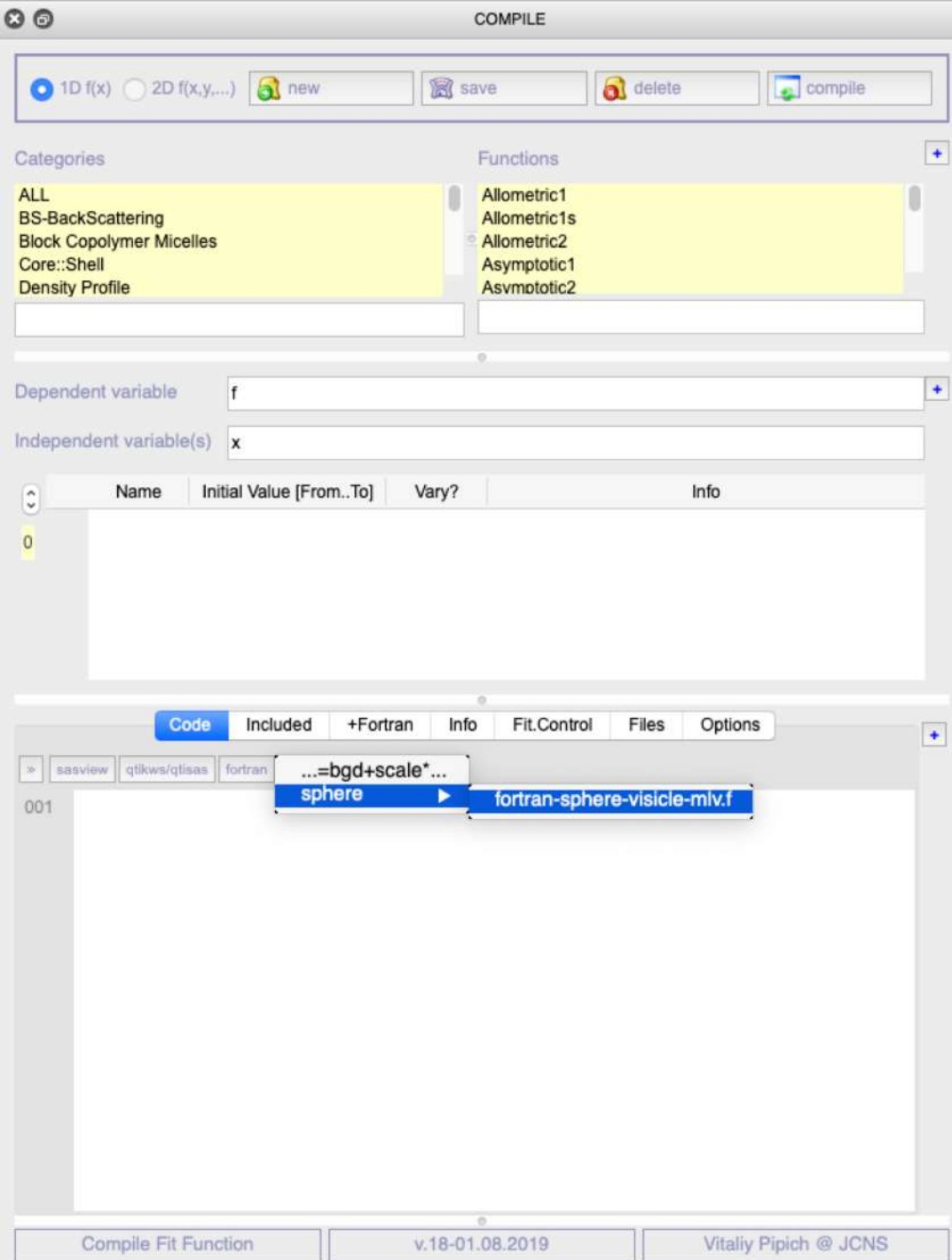
FIF-file: multilamellar-vesicle-model-hf.fif  
[move to "FitFunctions"]

# Example: Multilamellar Vesicle Model

```
th36_(&Q, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift,  
&bckgr)
```



Push „new“ button



- push „fortran“ button;
- select from menu needed Fortran file;
- to use Fortran file from “fortran” menu file should be prepared (see next pages);
- In example we selected “fortran-sphere-vesicle-mlv.f”

COMPILE

1D f(x) 2D f(x,y,...)

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Core:Shell, Density Profile

Functions: Allometric1, Allometric1s, Allometric2, Asymptotic1, Asymptotic2

Dependent variable: f

Independent variable(s): x

Code Included +Fortran Info Fit.Control Files Options

.../h36\_double...  
.../fortran-sphere-vesicle-mv1

COMPILE

1D f(x) 2D f(x,y,...)

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Core:Shell, Density Profile

Functions: Allometric1, Allometric1s, Allometric2, Asymptotic1, Asymptotic2

Dependent variable: f

Independent variable(s): x

Name	Initial Value [From..To]	Vary?	Info
1 phi	0.01[0.0..1.0]	<input type="checkbox"/>	[1] Konzentration Polymer
2 n	3[1..100]	<input type="checkbox"/>	[1] Anzahl der Schichten
3 nw	0.1[0.0..1.0]	<input type="checkbox"/>	[1] width of n-distribution

Code Included +Fortran Info Fit.Control Files Options

h36\_(&x, &phi, &n, &nw, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &backgr)

Compile Fit Function v.18-01.08.2019 Vitaliy Pipich @ JCMS

COMPILE

1D f(x) 2D f(x,y,...)

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Core:Shell, Density Profile

Functions: Allometric1, Allometric1s, Allometric2, Asymptotic1, Asymptotic2

Dependent variable: f

Independent variable(s): x

Name	Initial Value [From..To]	Vary?	Info
1 phi	0.01[0.0..1.0]	<input type="checkbox"/>	[1] Konzentration Polymer
2 n	3[1..100]	<input type="checkbox"/>	[1] Anzahl der Schichten
3 nw	0.1[0.0..1.0]	<input type="checkbox"/>	[1] width of n-distribution

Code Included +Fortran Info Fit.Control Files Options

Use FORTRAN functions from file:  
./IncludedFunctions/fortran-sphere-vesicle-mv1

Forward Declaration [FORTRAN functions in CPP]:

```
double h36_(double,double,double,double,double,double,double,double,double,double,double);
double invesicle4a_(double);
double invesicle4_(double,double);
double osz_(double,double);
double lgama_(double,double);
```

Compile Fit Function v.18-01.08.2019 Vitaliy Pipich @ JCMS

COMPILE

1D f(x) 2D f(x,y,...)

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Core:Shell, Density Profile

Functions: Allometric1, Allometric1s, Allometric2, Asymptotic1, Asymptotic2

Dependent variable: f

Independent variable(s): x

Name	Initial Value [From..To]	Vary?	Info
1 phi	0.01[0.0..1.0]	<input type="checkbox"/>	[1] Konzentration Polymer
2 n	3[1..100]	<input type="checkbox"/>	[1] Anzahl der Schichten
3 nw	0.1[0.0..1.0]	<input type="checkbox"/>	[1] width of n-distribution

Code Included +Fortran Info Fit.Control Files Options

h36\_(&x, &phi, &n, &nw, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &backgr)::  
Multilamellar vesicle model  
Model author: Henrich Frielinghaus  
<https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603>  
Fortran code: Henrich Frielinghaus  
tikws adaptation: Vitaliy Pipich  
Good place for function's comments

Compile Fit Function v.18-01.08.2019 Vitaliy Pipich @ JCMS

COMPILE

1D f(x) 2D f(x,y,...) new save delete compile

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Core-Shell, Density Profile

Functions: Alometric1, Alometric1s, Alometric2, Asymptotic1, Asymptotic2

Dependent variable: f

Independent variable(s): x

Name	Initial Value [From..To]	Vary?	Info
0			

COMPILE

1D f(x) 2D f(x,y,...) new save delete compile

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Cholesterol-lisosomes

Functions: muscatt-example-12t1, muscatt-example-12t2, muscatt-example-12t3

Dependent variable: y

Independent variable(s): x

Name	Initial Value	Vary?From..To	Info
1 ^ phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer
2 ^ n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten
3 ^ nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution

Code +Included +Fortran Info Fit.Control Files Options

```

234. y=#36_(&x, &phi, &n, &nw, &rhov, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr);
235.
236.
237.
  
```

COMPILE

1D f(x) 2D f(x,y,...) new save delete compile

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Cholesterol-lisosomes, Form Factors

Functions: multilamellar-vesicle-model-hf, muscatt, muscatt-example-12t1, multilamellar-vesicle-model-hf

Dependent variable: y

Independent variable(s): x

Name	Initial Value	Vary?From..To	Info
1 ^ phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer
2 ^ n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten
3 ^ nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution

Code +Included +Fortran Info Fit.Control Files Options

```

234. y=th36_(&x) &phi, &n, &nw, &rhov, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr);
235.
236.
237.
  
```

multilamellar-vesicle-model-hf

Results Log

```

<< compile >>
<< compile status >> OK: function 'multilamellar-vesicle-model-hf' is ready
  
```

fortran-sphere-vesicle-mlv.f

- Name of the file should start with "**fortran-**";

- Second word in the file name defines (here "**sphere**") sub-folder in the menu (see prev. page);

- File should be located in "**FitFunctions/IncludedFunctions**" folder;

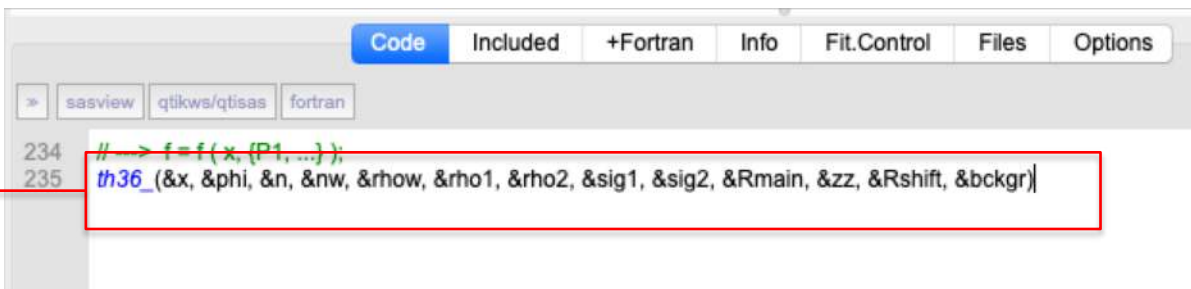
# Fortran file is “decorated“ with 7 lines of comments in the header (see below first 7 lines)

```
1 C[name] th36
2 C[parameter_names] phi, n, nw, rhoW, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9     function th36(x,xphi,xn,xnw,xrhoW,xrho1,xrho2,xsig1,xsig2,
10 *           xRmain,xzz,xRshift,xbckgr)
11
12 C
13 implicit none
14
15 C
16 double precision th36
17 double precision x
18
19 C
20 double precision Pi
21 parameter (Pi = 3.14159265358979323846264338328d0)
22
23 C
24 double precision xphi      ! Konzentration Polymer
25 double precision xn        ! Anzahl der Schichten
26 double precision xnw       ! width of n-distribution
27 double precision rhoW      ! SLD Wasser
28 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
29 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
30 double precision xRmain    ! Main Radius
31 double precision xzz       ! Z - Schultz distribution
32 double precision xRshift   ! Maximum possible shift
33 double precision xbckgr    ! background
34
35 C
36 double precision q        ! Q-Vektor
37 double precision phi      ! Konzentration Polymer
38 double precision n        ! Anzahl der Schichten
39 double precision nw       ! width of n-distribution
40 double precision rhoW      ! SLD Wasser
41 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
42 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
43 double precision Rmain    ! Main Radius
44 double precision zz       ! Z - Schultz distribution
45 double precision Rshift   ! Maximum possible shift
46 double precision bckgr    ! background
47
48 C
49 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
50
51 C
52 double precision bmin,bmax ! Integrationsgrenzen
53 double precision eps       ! Fehler
54 integer          maxit     ! Maximale Iterationen
```



Line #1 starts with **C[name]** and contains “main” Fortran function will be called from c-code of fitting function

```
1 C[name] th36
2 C[parameter_names] phi, n, nw, rhoW, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [1], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9 function th36(x,xphi,xn,xnw,xrhoW,xrho1,xrho2,xsig1,xsig2,
10 * xRmain,xzz,xRshift,xbckgr)
11
12 C
13 implicit none
14
15 C
16 double precision th36
17 double precision x
18
19 C
20 double precision Pi
21 parameter (Pi = 3.14159265358979323846264338328d0)
22
23 C
24 double precision xphi ! Konzentration Polymer
25 double precision xn ! Anzahl der Schichten
26 double precision xnw ! width of n-distribution
27 double precision rhoW ! SLD Wasser
28 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
29 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
30 double precision xRmain ! Main Radius
31 double precision xzz ! Z - Schultz distribution
32 double precision xRshift ! Maximum possible shift
33 double precision xbckgr ! background
34
35 C
36 double precision q ! Q-Vektor
37 double precision phi ! Konzentration Polymer
38 double precision n ! Anzahl der Schichten
39 double precision nw ! width of n-distribution
40 double precision rhoW ! SLD Wasser
41 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
42 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
43 double precision Rmain ! Main Radius
44 double precision zz ! Z - Schultz distribution
45 double precision Rshift ! Maximum possible shift
46 double precision bckgr ! background
47
48 C
49 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
50
51 C
52 double precision bmin,bmax ! Integrationsgrenzen
53 double precision eps ! Fehler
54 integer maxit ! Maximale Iterationen
```



Line #2 starts with **C[parameter\_name]** and contains list of parameter names separates by ,

```

1 C[name] th36
2 C[parameter_names] phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9
10 function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
11 * xRmain,xzz,xRshift,xbckgr)
12
13 implicit none
14
15 C
16 double precision th36
17 double precision x
18
19 double precision Pi
20 parameter (Pi = 3.141592653589793238462643383280)
21
22 C
23 double precision xphi ! Konzentration Polymer
24 double precision xn ! Anzahl der Schichten
25 double precision xnw ! width of n-distribution
26 double precision xrhoW ! SLD Wasser
27 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
28 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
29 double precision xRmain ! Main Radius
30 double precision xzz ! Z - Schultz distribution
31 double precision xRshift ! Maximum possible shift
32 double precision xbckgr ! background
33
34 C
35 double precision q ! Q-Vektor
36 double precision phi ! Konzentration Polymer
37 double precision n ! Anzahl der Schichten
38 double precision nw ! width of n-distribution
39 double precision rhoW ! SLD Wasser
40 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
41 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
42 double precision Rmain ! Main Radius
43 double precision zz ! Z - Schultz distribution
44 double precision Rshift ! Maximum possible shift
45 double precision bckgr ! background
46
47 C
48 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
49
50 C
51 double precision bmin,bmax ! Integrationsgrenzen
52 double precision eps ! Fehler
53 integer maxit ! Maximale Iterationen

```

Code Included +Fortran Info Fit.Control Files Options

> sasview qtikws/qtisas fortran

```

234 // --> f = f(x, (P1, ...));
235 th36 (&x, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr)

```

C	Name	Initial Value	Vary?From..To	Info
1 ^	phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer
2 ^	n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten
3 ^	nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution
4 ^	rhow	-5.6e+09	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD Wasser
5 ^	rho1	2e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der Dekoration (2)
7 ^	sig1	50	<input type="checkbox"/> 0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8 ^	sig2	20	<input type="checkbox"/> 0.0..10000	[A] Dicke der Dekoration (2)
9 ^	Rmain	800	<input type="checkbox"/> 0.0..100000.0	[A] Main Radius
10 ^	zz	0.2	<input type="checkbox"/> 0.0..10000	[?] Z - Schultz distribution
11 ^	Rshift	10	<input type="checkbox"/> 0.0..10000.0	[A] Maximum possible shift
12 ^	bckgr	0.01	<input type="checkbox"/> ..	[1/cm] background

Line #3 starts with **C[parameter\_init\_values]** and contains list of initial values of parameters separates by ,

```

1 C[name] th36
2 C[parameter_names] phi, n, nw, rhoW, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9 function th36(x,xphi,xn,xnw,xrhoW,xrho1,xrho2,xsig1,xsig2,
10 * xRmain,xzz,xRshift,xbckgr)
11
12 C
13 implicit none
14
15 C
16 double precision th36
17 double precision x
18
19 C
20 double precision Pi
21 parameter (Pi = 3.14159265358979323846264338328d0)
22
23 C
24 double precision xphi ! Konzentration Polymer
25 double precision xn ! Anzahl der Schichten
26 double precision xnw ! width of n-distribution
27 double precision rhoW ! SLD Wasser
28 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
29 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
30 double precision xRmain ! Main Radius
31 double precision xzz ! Z - Schultz distribution
32 double precision xRshift ! Maximum possible shift
33 double precision xbckgr ! background
34
35 C
36 double precision q ! Q-Vektor
37 double precision phi ! Konzentration Polymer
38 double precision n ! Anzahl der Schichten
39 double precision nw ! width of n-distribution
40 double precision rhoW ! SLD Wasser
41 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
42 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
43 double precision Rmain ! Main Radius
44 double precision zz ! Z - Schultz distribution
45 double precision Rshift ! Maximum possible shift
46 double precision bckgr ! background
47
48 C
49 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
50
51 C
52 double precision bmin,bmax ! Integrationsgrenzen
53 double precision eps ! Fehler
54 integer maxit ! Maximale Iterationen

```

Dependent variable		y			
Independent variable(s)		x			
	Name	Initial Value	Vary?From..To	Info	
1 ^	phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer	
2 ^	n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten	
3 ^	nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution	
4 ^	rhoW	-5.6e+09	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD Wasser	
5 ^	rho1	2e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)	
6 ^	rho2	3e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der Dekoration (2)	
7 ^	sig1	50	<input type="checkbox"/> 0.0..10000.0	[A] Dicke der zentralen Schicht (1)	
8 ^	sig2	20	<input type="checkbox"/> 0.0..10000	[A] Dicke der Dekoration (2)	
9 ^	Rmain	800	<input type="checkbox"/> 0.0..100000.0	[A] Main Radius	
10 ^	zz	0.2	<input type="checkbox"/> 0.0..10000	[?1] Z - Schultz distribution	
11 ^	Rshift	10	<input type="checkbox"/> 0.0..10000.0	[A] Maximum possible shift	
12 ^	bckgr	0.01	<input type="checkbox"/> ..	[1/cm] background	

Line #4 starts with **C[parameter\_init\_range]** and contains list of ranges of initial values of parameters separates by ,  
 In format "[left..right]"

```

1 C[name] th36
2 C[parameter_names] phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9 function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10 * xRmain,xzz,xRshift,xbckgr)
11
12 C
13 implicit none
14
15 double precision th36
16 double precision x
17
18 C
19 double precision Pi
20 parameter (Pi = 3.14159265358979323846264338328d0)
21
22 C
23 double precision xphi ! Konzentration Polymer
24 double precision xn ! Anzahl der Schichten
25 double precision xnw ! width of n-distribution
26 double precision xrhow ! SLD Wasser
27 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
28 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
29 double precision xRmain ! Main Radius
30 double precision xzz ! Z - Schultz distribution
31 double precision xRshift ! Maximum possible shift
32 double precision xbckgr ! background
33
34 C
35 double precision q ! Q-Vektor
36 double precision phi ! Konzentration Polymer
37 double precision n ! Anzahl der Schichten
38 double precision nw ! width of n-distribution
39 double precision rhoW ! SLD Wasser
40 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
41 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
42 double precision Rmain ! Main Radius
43 double precision zz ! Z - Schultz distribution
44 double precision Rshift ! Maximum possible shift
45 double precision bckgr ! background
46
47 C
48 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
49
50 C
51 double precision bmin,bmax ! Integrationsgrenzen
52 double precision eps ! Fehler
53 integer maxit ! Maximale Iterationen
  
```

Dependent variable		y		
Independent variable(s)		x		
	Name	Initial Value	Vary?From..To	Info
1 ^	phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer
2 ^	n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten
3 ^	nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution
4 ^	rhow	-5.6e+09	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD Wasser
5 ^	rho1	2e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der Dekoration (2)
7 ^	sig1	50	<input type="checkbox"/> 0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8 ^	sig2	20	<input type="checkbox"/> 0.0..10000	[A] Dicke der Dekoration (2)
9 ^	Rmain	800	<input type="checkbox"/> 0.0..100000.0	[A] Main Radius
10 ^	zz	0.2	<input type="checkbox"/> 0.0..10000	[?1] Z - Schultz distribution
11 ^	Rshift	10	<input type="checkbox"/> 0.0..10000.0	[A] Maximum possible shift
12 ^	bckgr	0.01	<input type="checkbox"/> ..	[1/cm] background

Line #5 starts with **C[parameter\_units]** and contains list of units of parameters separates by ,  
 In format "**[UNITS]**"

```

1 C[name] th36
2 C[parameter_names] phi_n_nw_rhoW_rho1_rho2_sig1_sig2_Rmain_zz_Rshift_bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9 function th36(x,xphi,xn,xnw,xrhoW,xrho1,xrho2,xsig1,xsig2,
10 * xRmain,xzz,xRshift,xbckgr)
11
12 C
13 implicit none
14
15 C
16 double precision th36
17 double precision x
18
19 C
20 double precision Pi
21 parameter (Pi = 3.141592653589793238462643383280)
22
23 C
24 double precision xphi ! Konzentration Polymer
25 double precision xn ! Anzahl der Schichten
26 double precision xnw ! width of n-distribution
27 double precision xrhoW ! SLD Wasser
28 double precision xrho1,xrho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
29 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
30 double precision xRmain ! Main Radius
31 double precision xzz ! Z - Schultz distribution
32 double precision xRshift ! Maximum possible shift
33 double precision xbckgr ! background
34
35 C
36 double precision q ! Q-Vektor
37 double precision phi ! Konzentration Polymer
38 double precision n ! Anzahl der Schichten
39 double precision nw ! width of n-distribution
40 double precision rhoW ! SLD Wasser
41 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
42 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
43 double precision Rmain ! Main Radius
44 double precision zz ! Z - Schultz distribution
45 double precision Rshift ! Maximum possible shift
46 double precision bckgr ! background
47
48 C
49 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
50
51 C
52 double precision bmin,bmax ! Integrationsgrenzen
53 double precision eps ! Fehler
54 integer maxit ! Maximale Iterationen
  
```

Dependent variable		y			
Independent variable(s)		x			
	Name	Initial Value	Vary?From..To	Info	
1 ^	phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer	
2 ^	n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten	
3 ^	nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution	
4 ^	rhoW	-5.6e+09	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD Wasser	
5 ^	rho1	2e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)	
6 ^	rho2	3e+10	<input type="checkbox"/> -1e10..10e10	[1/cm^2] SLD der Dekoration (2)	
7 ^	sig1	50	<input type="checkbox"/> 0.0..10000.0	[A] Dicke der zentralen Schicht (1)	
8 ^	sig2	20	<input type="checkbox"/> 0.0..10000	[A] Dicke der Dekoration (2)	
9 ^	Rmain	800	<input type="checkbox"/> 0.0..10000.0	[A] Main Radius	
10 ^	zz	0.2	<input type="checkbox"/> 0.0..10000	[?1] Z - Schultz distribution	
11 ^	Rshift	10	<input type="checkbox"/> 0.0..10000.0	[A] Maximum possible shift	
12 ^	bckgr	0.01	<input type="checkbox"/> ..	[1/cm] background	

Line #6 starts with **C[parameter\_info]** and contains list of descriptions of parameters separates by ,  
 In format "[INFO...]"

```

1 C[name] th36
2 C[parameter_names] phi, n, nw, rhoW, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000.0], [0.0..100000.0], [0.0..10000.0], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9
10 function th36(x,xphi,xn,xnw,xrhoW,xrho1,xrho2,xsig1,xsig2,
11 *
12   xRmain,xzz,xRshift,xbckgr)
13
14 C
15 implicit none
16
17 C
18 double precision th36
19 double precision x
20
21 C
22 double precision Pi
23 parameter (Pi = 3.14159265358979323846264338328d0)
24
25 C
26 double precision xphi      ! Konzentration Polymer
27 double precision xn        ! Anzahl der Schichten
28 double precision xnw       ! width of n-distribution
29 double precision rhoW      ! SLD Wasser
30 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
31 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
32 double precision xRmain    ! Main Radius
33 double precision xzz       ! Z - Schultz distribution
34 double precision xRshift   ! Maximum possible shift
35 double precision xbckgr    ! background
36
37 C
38 double precision q        ! Q-Vektor
39 double precision phi      ! Konzentration Polymer
40 double precision n        ! Anzahl der Schichten
41 double precision nw       ! width of n-distribution
42 double precision rhoW     ! SLD Wasser
43 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
44 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
45 double precision Rmain    ! Main Radius
46 double precision zz       ! Z - Schultz distribution
47 double precision Rshift   ! Maximum possible shift
48 double precision bckgr    ! background
49
50 C
51 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
52
53 C
54 double precision bmin,bmax ! Integrationsgrenzen
55 double precision eps       ! Fehler
56 integer maxit             ! Maximale Iterationen
  
```

Dependent variable		y		
Independent variable(s)		x		
	Name	Initial Value	Vary?From..To	Info
1	phi	0.01	<input type="checkbox"/> 0.0..1.0	[1] Konzentration Polymer
2	n	3	<input type="checkbox"/> 1..100	[1] Anzahl der Schichten
3	nw	0.1	<input type="checkbox"/> 0.0..1.0	[1] width of n-distribution
4	rhoW	-5.6e+09	<input type="checkbox"/> -1e10..10e10	[1,cm^2] SLD Wasser
5	rho1	2e+10	<input type="checkbox"/> -1e10..10e10	[1,cm^2] SLD der zentralen Schicht (1)
6	rho2	3e+10	<input type="checkbox"/> -1e10..10e10	[1,cm^2] SLD der Dekoration (2)
7	sig1	50	<input type="checkbox"/> 0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8	sig2	20	<input type="checkbox"/> 0.0..10000.0	[A] Dicke der Dekoration (2)
9	Rmain	800	<input type="checkbox"/> 0.0..100000.0	[A] Main Radius
10	zz	0.2	<input type="checkbox"/> 0.0..10000.0	[?] Z - Schultz distribution
11	Rshift	10	<input type="checkbox"/> 0.0..10000.0	[A] Maximum possible shift
12	bckgr	0.01	<input type="checkbox"/> ..	[1,cm] background

Line #7 starts with **C[info]** and contains information about function. Every line is separated by „

```
1 C[name] th36
2 C[parameter_names] phi, n, nw, rhoW, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3 C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4 C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5 C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6 C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7 C[info] "Multilamellar vesicle model", "Model author: Henrich Frielinghaus", "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603", "Fortran code: Henrich Frielinghaus", "qtikws adaptation: Vitaliy Pipich"
8
9 function th36(x,xphi,xn,xnw,xrhoW,xrho1,xrho2,xsig1,xsig2,
10 * xRmain,xzz,xRshift,xbckgr)
11 C
12 implicit none
13 C
14 double precision th36
15 double precision x
16 C
17 double precision Pi
18 parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20 double precision xphi ! Konzentration Polymer
21 double precision xn ! Anzahl der Schichten
22 double precision xnw ! width of n-distribution
23 double precision rhoW ! SLD Wasser
24 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
25 double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26 double precision xRmain ! Main Radius
27 double precision xzz ! Z - Schultz distribution
28 double precision xRshift ! Maximum possible shift
29 double precision xbckgr ! background
30 C
31 double precision q ! Q-Vektor
32 double precision phi ! Konzentration Polymer
33 double precision n ! Anzahl der Schichten
34 double precision nw ! width of n-distribution
35 double precision rhoW ! SLD Wasser
36 double precision rho1,rho2 ! SLD der zentralen Schicht (1) und Dekoration (2)
37 double precision sig1,sig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
38 double precision Rmain ! Main Radius
39 double precision zz ! Z - Schultz distribution
40 double precision Rshift ! Maximum possible shift
41 double precision bckgr ! background
42 C
43 double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zur
44 C
45 double precision bmin,bmax ! Integrationsgrenzen
46 double precision eps ! Fehler
47 integer maxit ! Maximale Iterationen
```

Code	+Included	+Fortran	Info	Fit.Control	Files	Options
th36_(&x, &phi, &n, &nw, &rhoW, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr)::						
Multilamellar vesicle model						
Model author: Henrich Frielinghaus						
<a href="https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603">https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603</a>						
Fortran code: Henrich Frielinghaus						
qtikws/qtisas adaptation: Vitaliy Pipich						
v. 2021-03-10						