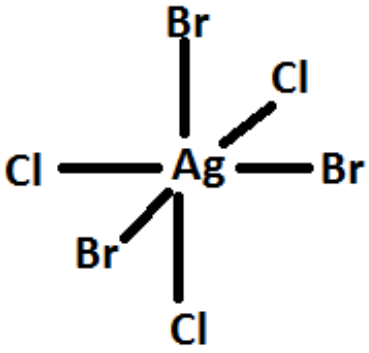
Determinando a distribuição dos ânions ao redor da Ag

Analisando o espectro na borda k da Ag

1- Considerando um arranjo facial



Arranjo dos átomos de Br e Cl na primeira esfera considerando uma isomeria facial

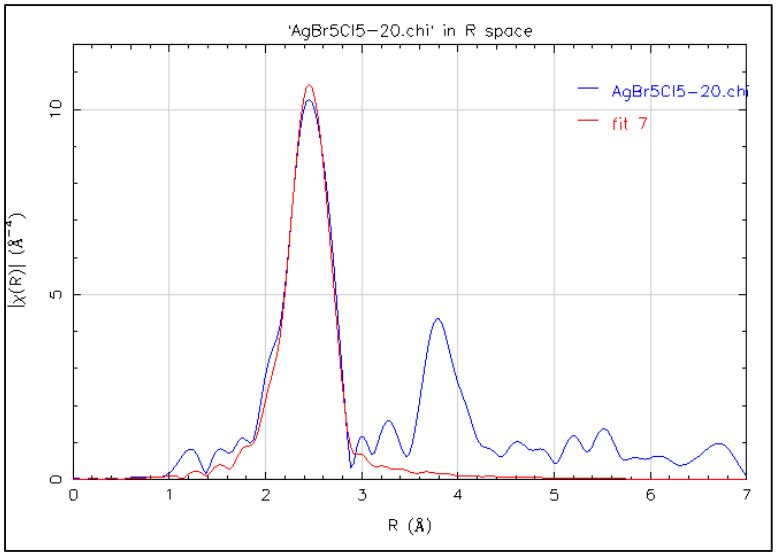
```
* ------------------------------------------------------------------
* The following crystallographic data were used:
*
* title        ...
* space = F m -3 m
* a =     5.66040        b =       5.66040        c =       5.66040
* alpha =       90.0    beta =    90.0    gamma =  90.0
* core =        Ag      edge =   K
* atoms
* ! elem    x           y           z       tag         occ
*   Ag     0.00000     0.00000     0.00000  Ag            1.00000
*   Br     0.50000     0.50000     0.50000  Br            1.00000
* ------------------------------------------------------------------
```

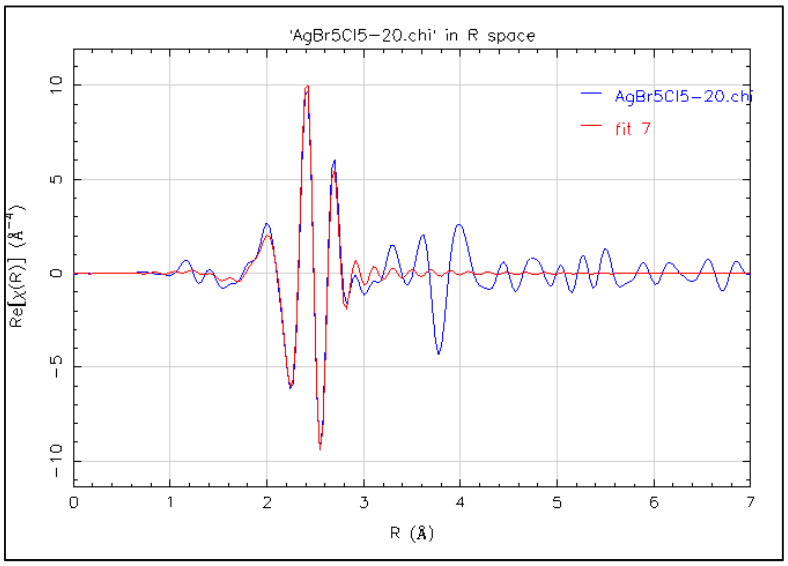
```
POTENTIALS
*    ipot   z  element
       0   47   Ag
       1   47   Ag
       2   35   Br
       3   17   Cl

ATOMS                          * this list contains 33 atoms
*   x          y          z       ipot  tag              distance
   0.00000    0.00000    0.00000  0 Ag              0.00000
   2.83020    0.00000    0.00000  3 Cl_1            2.83020
  -2.83020    0.00000    0.00000  2 Br_1            2.83020
   0.00000    2.83020    0.00000  3 Cl_1            2.83020
   0.00000   -2.83020    0.00000  2 Br_1            2.83020
   0.00000    0.00000    2.83020  3 Cl_1            2.83020
   0.00000    0.00000   -2.83020  2 Br_1            2.83020
   2.83020    2.83020    0.00000  1 Ag_1            4.00251
  -2.83020    2.83020    0.00000  1 Ag_1            4.00251
   2.83020   -2.83020    0.00000  1 Ag_1            4.00251
  -2.83020   -2.83020    0.00000  1 Ag_1            4.00251
   2.83020    0.00000    2.83020  1 Ag_1            4.00251
  -2.83020    0.00000    2.83020  1 Ag_1            4.00251
   0.00000    2.83020    2.83020  1 Ag_1            4.00251
   0.00000   -2.83020    2.83020  1 Ag_1            4.00251
   2.83020    0.00000   -2.83020  1 Ag_1            4.00251
  -2.83020    0.00000   -2.83020  1 Ag_1            4.00251
   0.00000    2.83020   -2.83020  1 Ag_1            4.00251
   0.00000   -2.83020   -2.83020  1 Ag_1            4.00251
   2.83020    2.83020    2.83020  2 Br_2            4.90205
  -2.83020    2.83020    2.83020  2 Br_2            4.90205
   2.83020   -2.83020    2.83020  2 Br_2            4.90205
  -2.83020   -2.83020    2.83020  2 Br_2            4.90205
   2.83020    2.83020   -2.83020  2 Br_2            4.90205
  -2.83020    2.83020   -2.83020  2 Br_2            4.90205
   2.83020   -2.83020   -2.83020  2 Br_2            4.90205
  -2.83020   -2.83020   -2.83020  2 Br_2            4.90205
   5.66040    0.00000    0.00000  1 Ag_2            5.66040
  -5.66040    0.00000    0.00000  1 Ag_2            5.66040
   0.00000    5.66040    0.00000  1 Ag_2            5.66040
   0.00000   -5.66040    0.00000  1 Ag_2            5.66040
   0.00000    0.00000    5.66040  1 Ag_2            5.66040
   0.00000    0.00000   -5.66040  1 Ag_2            5.66040
END
```

1	3	2.830	100.00		[+] Br_1 [+]
2	3	2.830	96.86		[+] Cl_1 [+]
3	12	4.003	100.00		[+] Ag_1 [+]
5	24	4.832	10.45		[+] Ag_1 Br_1 [+]
6	24	4.832	8.19		[+] Ag_1 Cl_1 [+]
7	4	4.902	14.47		[+] Br_2 [+]
8	4	4.902	11.30		[+] Cl_2 [+]
9	6	5.660	16.23		[+] Ag_2 [+]
10	6	5.660	3.72		[+] Cl_1 Br_1 [+]
11	6	5.660	33.58	1	[+] Ag_2 Br_1 [+]
12	6	5.660	29.48	1	[+] Ag_2 Cl_1 [+]
13	6	5.660	6.08	1	[+] Cl_1 [+] Br_1 [+]
16	3	5.660	34.98	2	[+] Br_1 Ag_2 Br_1 [+]
17	3	5.660	26.49	2	[+] Cl_1 Ag_2 Cl_1 [+]
23	24	5.867	2.96		[+] Cl_2 Ag_1 [+]

label:	
N:	3
S02:	amp*(1-x)
delE0:	enot
delR:	delr1
sigma^2:	ss1
Ei:	
3rd:	
4th:	

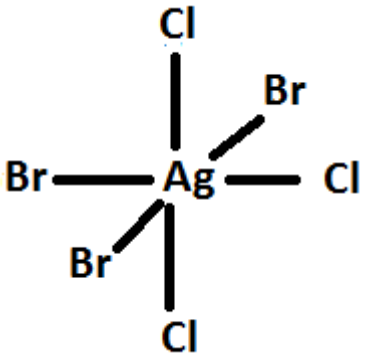
label:	
N:	3
S02:	amp*x
delE0:	enot
delR:	delr2
sigma^2:	ss2
Ei:	
3rd:	
4th:	






```
Independent points           =      16.075195312
Number of variables          =       6.000000000
Chi-square                   =    1631.398182579
Reduced Chi-square           =     161.922238922
R-factor                     =       0.000127532
Measurement uncertainty (k)  =       0.000060473
Measurement uncertainty (R)  =       0.033406205
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =      0.7288650   +/-       3.0480170     (0.0000)
  delr1            =      0.0361500   +/-       0.0112550     (0.0000)
  ss1              =      0.0019880   +/-       0.0006060     (0.0030)
  delr2            =     -0.1228670   +/-       0.0178020     (0.0000)
  ss2              =      0.0011920   +/-       0.0004710     (0.0030)
  x                =      0.5057740   +/-       0.1306190     (0.5000)

Set parameters:
  amp              =  0.9
```

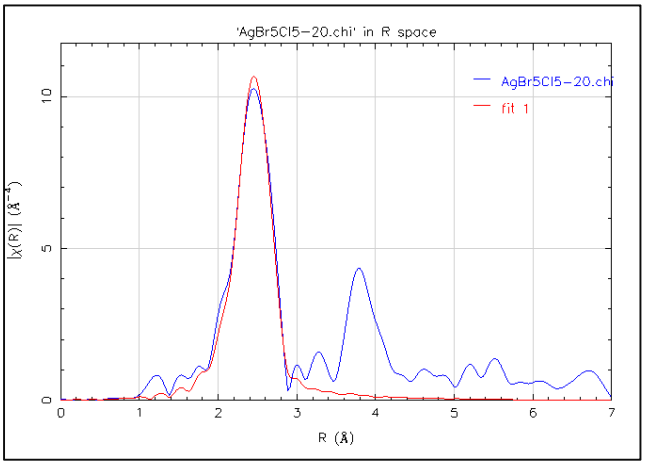
2- Considerando um arranjo meridional

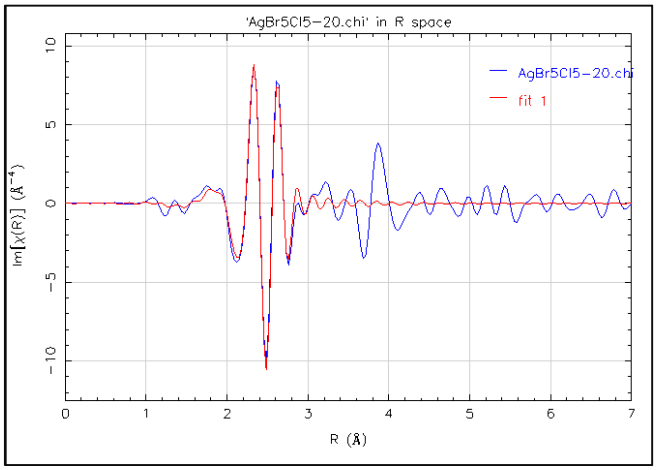


Arranjo dos átomos de Br e Cl na primeira esfera considerando uma isomeria meridional

```
POTENTIALS
*    ipot   Z  element
       0   47   Ag
       1   47   Ag
       2   35   Br
       3   17   Cl

ATOMS                                  * this list contains 33 atoms
*    x          y          z          ipot  tag              distance
    0.00000    0.00000    0.00000    0 Ag                   0.00000
    2.83020    0.00000    0.00000    2 Br_1                 2.83020
   -2.83020    0.00000    0.00000    2 Br_1                 2.83020
    0.00000    2.83020    0.00000    2 Br_1                 2.83020
    0.00000   -2.83020    0.00000    3 Cl_1                 2.83020
    0.00000    0.00000    2.83020    3 Cl_1                 2.83020
    0.00000    0.00000   -2.83020    3 Cl_1                 2.83020
    2.83020    2.83020    0.00000    1 Ag_1                 4.00251
   -2.83020    2.83020    0.00000    1 Ag_1                 4.00251
    2.83020   -2.83020    0.00000    1 Ag_1                 4.00251
   -2.83020   -2.83020    0.00000    1 Ag_1                 4.00251
    2.83020    0.00000    2.83020    1 Ag_1                 4.00251
   -2.83020    0.00000    2.83020    1 Ag_1                 4.00251
    0.00000    2.83020    2.83020    1 Ag_1                 4.00251
    0.00000   -2.83020    2.83020    1 Ag_1                 4.00251
    2.83020    0.00000   -2.83020    1 Ag_1                 4.00251
   -2.83020    0.00000   -2.83020    1 Ag_1                 4.00251
    0.00000    2.83020   -2.83020    1 Ag_1                 4.00251
    0.00000   -2.83020   -2.83020    1 Ag_1                 4.00251
```

1	3	2.830	100.00		[+] Br_1 [+]
2	3	2.830	96.37		[+] Cl_1 [+]
3	12	4.003	100.00		[+] Ag_1 [+]
5	24	4.832	10.08		[+] Ag_1 Br_1 [+]
6	24	4.832	7.86		[+] Ag_1 Cl_1 [+]
7	4	4.902	14.04		[+] Br_2 [+]
8	4	4.902	10.89		[+] Cl_2 [+]
9	6	5.660	16.25		[+] Ag_2 [+]
13	6	5.660	33.45	1	[+] Ag_2 Br_1 [+]
14	6	5.660	29.20	1	[+] Ag_2 Cl_1 [+]
15	2	5.660	3.09	1	[+] Br_1 [+] Br_1 [+]
20	3	5.660	34.76	2	[+] Br_1 Ag_2 Br_1 [+]
21	3	5.660	26.03	2	[+] Cl_1 Ag_2 Cl_1 [+]
29	24	5.867	2.93		[+] Cl_2 Ag_1 [+]





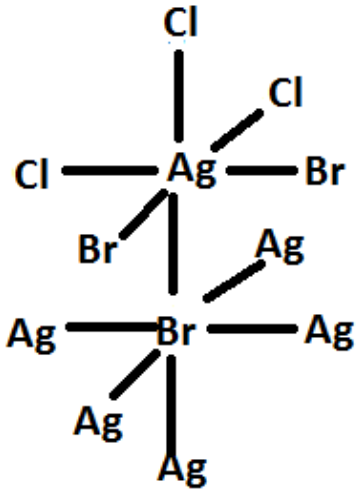

```
Independent points           =      15.802734375
Number of variables          =       6.000000000
Chi-square                   =    1492.488861382
Reduced Chi-square           =     152.252300663
R-factor                     =       0.000116727
Measurement uncertainty (k)  =       0.000060473
Measurement uncertainty (R)  =       0.033406205
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =      0.4845650   +/-       3.0282620     (0.0000)
  delr1            =      0.0353500   +/-       0.0111930     (0.0000)
  ss1              =      0.0018840   +/-       0.0006220     (0.0030)
  delr2            =     -0.1242920   +/-       0.0177610     (0.0000)
  ss2              =      0.0012070   +/-       0.0004650     (0.0030)
  x                =      0.5132420   +/-       0.1279800     (0.5000)

Set parameters:
  amp              =  0.9
```

Resumo dos resultados do ajuste da primeira vizinhança para o arranjo facial e meridional

Arranjo dos ânions	**Enot**	**r (Å)**		**Sigma^2 (10^{-3})**		**Delta r**		**Fração mássica (x)**
		Br	**Cl**	ss1	ss2	Delr1	Delr2	
Facial	0.73	2.86	2,70	1.98±0.60	1.19±0.47	0.036±0.011	-0.123±0.018	0.51±0.13
Meridiano	0.48	2,86	2,70	1.88±0.62	1.21±0.46	0.035±0.011	-0.124±0.018	0.51±0.12

Tratando os espectros na borda k da Ag e do Br simultaneamente

1- Considerando um arranjo facial




```
POTENTIALS
*    ipot   z  element
       0   47   Ag
       1   47   Ag
       2   35   Br
       3   17   Cl

ATOMS                          * this list contains 57 atoms
*    x          y          z       ipot  tag          distance
    0.00000    0.00000    0.00000    0 Ag           0.00000
    2.88725    0.00000    0.00000    2 Br_1         2.88725
   -2.88725    0.00000    0.00000    3 Cl_1         2.88725
    0.00000    2.88725    0.00000    2 Br_1         2.88725
    0.00000   -2.88725    0.00000    3 Cl_1         2.88725
    0.00000    0.00000    2.88725    3 Cl_1         2.88725
    0.00000    0.00000   -2.88725    2 Br_1         2.88725
    2.88725    2.88725    0.00000    1 Ag_1         4.08319
   -2.88725    2.88725    0.00000    1 Ag_1         4.08319
    2.88725   -2.88725    0.00000    1 Ag_1         4.08319
   -2.88725   -2.88725    0.00000    1 Ag_1         4.08319
    2.88725    0.00000    2.88725    1 Ag_1         4.08319
   -2.88725    0.00000    2.88725    1 Ag_1         4.08319
    0.00000    2.88725    2.88725    1 Ag_1         4.08319
    0.00000   -2.88725    2.88725    1 Ag_1         4.08319
    2.88725    0.00000   -2.88725    1 Ag_1         4.08319
   -2.88725    0.00000   -2.88725    1 Ag_1         4.08319
    0.00000    2.88725   -2.88725    1 Ag_1         4.08319
    0.00000   -2.88725   -2.88725    1 Ag_1         4.08319
    2.88725    2.88725    2.88725    2 Br_2         5.00086
   -2.88725    2.88725    2.88725    2 Br_2         5.00086
    2.88725   -2.88725    2.88725    2 Br_2         5.00086
```

```
POTENTIALS
*    ipot   z  element
       0   35   Br
       1   35   Br
       2   47   Ag

ATOMS                          * this list contains 57 atoms
*    x          y          z       ipot  tag          distance
    0.00000    0.00000    0.00000    0 Br           0.00000
    2.88725    0.00000    0.00000    2 Ag_1         2.88725
   -2.88725    0.00000    0.00000    2 Ag_1         2.88725
    0.00000    2.88725    0.00000    2 Ag_1         2.88725
    0.00000   -2.88725    0.00000    2 Ag_1         2.88725
    0.00000    0.00000    2.88725    2 Ag_1         2.88725
    0.00000    0.00000   -2.88725    2 Ag_1         2.88725
    2.88725    2.88725    0.00000    1 Br_1         4.08319
   -2.88725    2.88725    0.00000    1 Br_1         4.08319
    2.88725   -2.88725    0.00000    1 Br_1         4.08319
   -2.88725   -2.88725    0.00000    1 Br_1         4.08319
    2.88725    0.00000    2.88725    1 Br_1         4.08319
   -2.88725    0.00000    2.88725    1 Br_1         4.08319
    0.00000    2.88725    2.88725    1 Br_1         4.08319
    0.00000   -2.88725    2.88725    1 Br_1         4.08319
    2.88725    0.00000   -2.88725    1 Br_1         4.08319
   -2.88725    0.00000   -2.88725    1 Br_1         4.08319
    0.00000    2.88725   -2.88725    1 Br_1         4.08319
    0.00000   -2.88725   -2.88725    1 Br_1         4.08319
    2.88725    2.88725    2.88725    2 Ag_2         5.00086
   -2.88725    2.88725    2.88725    2 Ag_2         5.00086
```

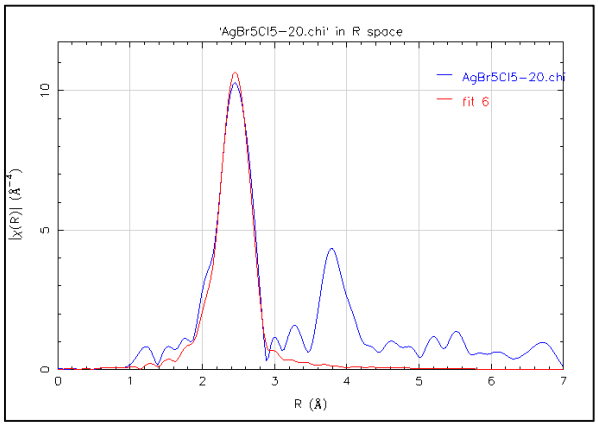
1	3	2.887	100.00		[+] Br_1 [+]
2	3	2.887	100.00		[+] Cl_1 [+]
3	12	4.083	100.00		[+] Ag_1 [+]
4	24	4.929	8.98		[+] Ag_1 Br_1 [+]
5	24	4.929	7.17		[+] Ag_1 Cl_1 [+]
6	8	5.001	26.06		[+] Br_2 [+]
7	6	5.774	16.07		[+] Ag_2 [+]
8	6	5.774	3.30		[+] Cl_1 Br_1 [+]
9	6	5.774	31.08	1	[+] Ag_2 Br_1 [+]
10	6	5.774	28.47	1	[+] Ag_2 Cl_1 [+]
11	6	5.774	5.29	1	[+] Cl_1 [+] Br_1 [+]
14	3	5.774	30.14	2	[+] Br_1 Ag_2 Br_1 [+]
15	3	5.774	25.11	2	[+] Cl_1 Ag_2 Cl_1 [+]
18	24	5.986	2.69		[+] Br_2 Br_1 [+]
20	48	5.986	4.20		[+] Br_2 Ag_1 [+]
21	48	6.125	3.89		[+] Ag_1 Ag_1 [+]

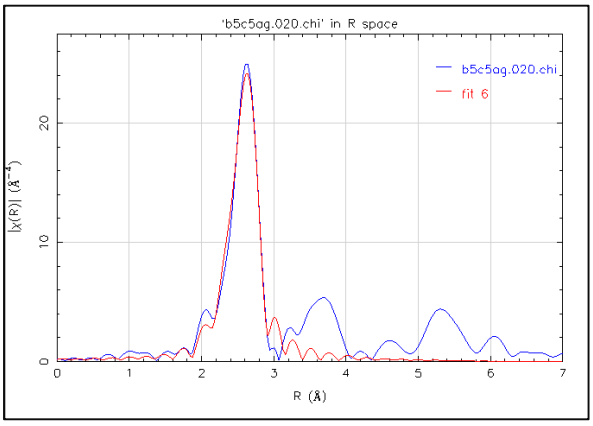
1	6	2.887	100.00		[+] Ag_1 [+]
2	12	4.083	72.39		[+] Br_1 [+]
3	48	4.929	13.76		[+] Br_1 Ag_1 [+]
4	8	5.001	32.25		[+] Ag_2 [+]
5	6	5.774	13.54		[+] Br_2 [+]
6	6	5.774	7.56		[+] Ag_1 Ag_1 [+]
7	12	5.774	42.56	1	[+] Br_2 Ag_1 [+]
8	6	5.774	13.35	1	[+] Ag_1 [+] Ag_1 [+]
9	6	5.774	2.87		[+] Ag_1 [+] Ag_1 [+]
10	6	5.774	41.53	2	[+] Ag_1 Br_2 Ag_1 [+]
13	48	5.986	4.74		[+] Br_1 Ag_1 [+]
14	48	5.986	5.38		[+] Ag_2 Ag_1 [+]
15	48	5.986	9.90		[+] Ag_2 Br_1 [+]
16	48	6.125	6.29		[+] Br_1 Br_1 [+]
17	24	6.456	44.41		[+] Ag_3 [+]

label:	
N:	3
S02:	amp*(1-x)
delE0:	enot_Ag
delR:	delr1
sigma^2:	ss1
Ei:	
3rd:	
4th:	

label:	
N:	3
S02:	amp*x
delE0:	enot_Ag
delR:	delr2
sigma^2:	ss2
Ei:	
3rd:	
4th:	

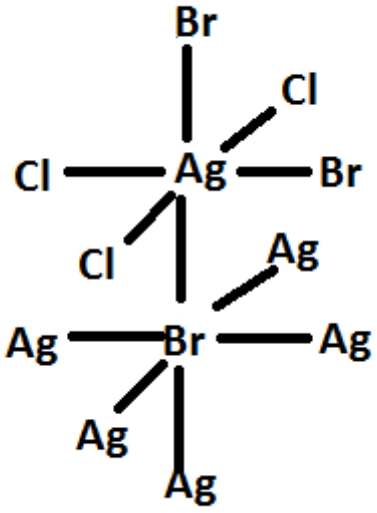
label:	
N:	6
S02:	amp
delE0:	enot_Br
delR:	delr3
sigma^2:	ss3
Ei:	
3rd:	
4th:	






```
Independent points           =      32.695312500
Number of variables          =       9.000000000
Chi-square                   =   10741.822449526
Reduced Chi-square           =     453.331115575
R-factor                     =       0.000101615
Measurement uncertainty (k)  =       0.000082258
Measurement uncertainty (R)  =       0.045440538
Number of data sets          =       2.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot_Ag          =      0.6702960   +/-      5.0365360     (0.0000)
  delr1            =     -0.0203880   +/-      0.0187480     (0.0000)
  ss1              =      0.0016850   +/-      0.0009470     (0.0030)
  enot_Br          =      3.3653260   +/-      0.7029760     (0.0000)
  delr2            =     -0.1801350   +/-      0.0292470     (0.0000)
  ss2              =      0.0008380   +/-      0.0008000     (0.0030)
  delr3            =     -0.0567080   +/-      0.0027450     (0.0000)
  ss3              =      0.0048650   +/-      0.0000780     (0.0030)
  x                =      0.4934070   +/-      0.2195300     (0.5000)

Set parameters:
  amp              =  0.9
```

2- Considerando um arranjo meridional



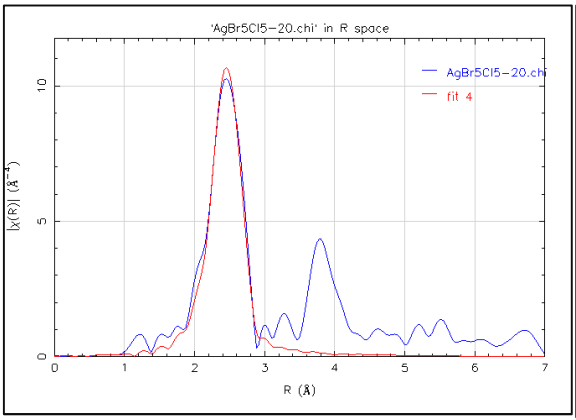

```
POTENTIALS
*    ipot   Z  element
       0   47   Ag
       1   47   Ag
       2   35   Br
       3   17   Cl

ATOMS                                  * this list contains 57 atoms
*   x          y          z       ipot  tag              distance
   0.00000    0.00000    0.00000   0 Ag                 0.00000
   2.88725    0.00000    0.00000   2 Br_1               2.88725
  -2.88725    0.00000    0.00000   3 Cl_1               2.88725
   0.00000    2.88725    0.00000   3 Cl_1               2.88725
   0.00000   -2.88725    0.00000   3 Cl_1               2.88725
   0.00000    0.00000    2.88725   2 Br_1               2.88725
   0.00000    0.00000   -2.88725   2 Br_1               2.88725
   2.88725    2.88725    0.00000   1 Ag_1               4.08319
  -2.88725    2.88725    0.00000   1 Ag_1               4.08319
   2.88725   -2.88725    0.00000   1 Ag_1               4.08319
  -2.88725   -2.88725    0.00000   1 Ag_1               4.08319
   2.88725    0.00000    2.88725   1 Ag_1               4.08319
  -2.88725    0.00000    2.88725   1 Ag_1               4.08319
   0.00000    2.88725    2.88725   1 Ag_1               4.08319
   0.00000   -2.88725    2.88725   1 Ag_1               4.08319
   2.88725    0.00000   -2.88725   1 Ag_1               4.08319
  -2.88725    0.00000   -2.88725   1 Ag_1               4.08319
   0.00000    2.88725   -2.88725   1 Ag_1               4.08319
   0.00000   -2.88725   -2.88725   1 Ag_1               4.08319
   2.88725    2.88725    2.88725   2 Br_2               5.00086
```

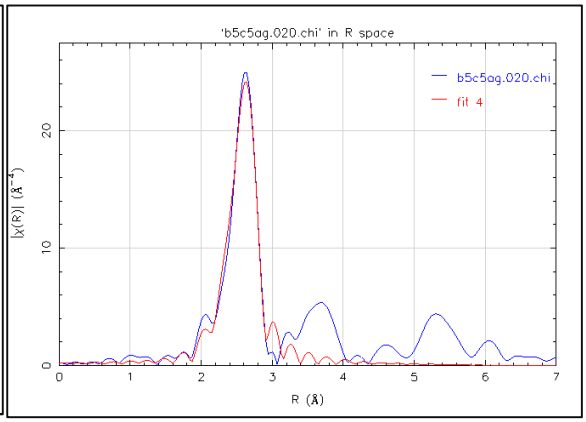
```
POTENTIALS
*    ipot   Z  element
       0   35   Br
       1   35   Br
       2   47   Ag

ATOMS                                  * this list contains 57 atoms
*   x          y          z       ipot  tag              distance
   0.00000    0.00000    0.00000   0 Br                 0.00000
   2.88725    0.00000    0.00000   2 Ag_1               2.88725
  -2.88725    0.00000    0.00000   2 Ag_1               2.88725
   0.00000    2.88725    0.00000   2 Ag_1               2.88725
   0.00000   -2.88725    0.00000   2 Ag_1               2.88725
   0.00000    0.00000    2.88725   2 Ag_1               2.88725
   0.00000    0.00000   -2.88725   2 Ag_1               2.88725
   2.88725    2.88725    0.00000   1 Br_1               4.08319
  -2.88725    2.88725    0.00000   1 Br_1               4.08319
   2.88725   -2.88725    0.00000   1 Br_1               4.08319
  -2.88725   -2.88725    0.00000   1 Br_1               4.08319
   2.88725    0.00000    2.88725   1 Br_1               4.08319
  -2.88725    0.00000    2.88725   1 Br_1               4.08319
   0.00000    2.88725    2.88725   1 Br_1               4.08319
   0.00000   -2.88725    2.88725   1 Br_1               4.08319
   2.88725    0.00000   -2.88725   1 Br_1               4.08319
  -2.88725    0.00000   -2.88725   1 Br_1               4.08319
   0.00000    2.88725   -2.88725   1 Br_1               4.08319
   0.00000   -2.88725   -2.88725   1 Br_1               4.08319
   2.88725    2.88725    2.88725   2 Ag_2               5.00086
  -2.88725    2.88725    2.88725   2 Ag_2               5.00086
```

1	3	2.887	100.00		[+] Br_1 [+]
2	3	2.887	100.00		[+] Cl_1 [+]
3	12	4.083	100.00		[+] Ag_1 [+]
5	24	4.929	9.02		[+] Ag_1 Br_1 [+]
6	24	4.929	7.20		[+] Ag_1 Cl_1 [+]
7	8	5.001	26.22		[+] Br_2 [+]
8	6	5.774	16.07		[+] Ag_2 [+]
12	6	5.774	31.20	1	[+] Ag_2 Br_1 [+]
13	6	5.774	28.55	1	[+] Ag_2 Cl_1 [+]
19	3	5.774	30.38	2	[+] Br_1 Ag_2 Br_1 [+]
20	3	5.774	25.25	2	[+] Cl_1 Ag_2 Cl_1 [+]
23	24	5.986	2.71		[+] Br_2 Br_1 [+]

1	6	2.887	100.00		[+] Ag_1 [+]
2	12	4.083	72.39		[+] Br_1 [+]
3	48	4.929	13.76		[+] Br_1 Ag_1 [+]
4	8	5.001	32.25		[+] Ag_2 [+]
5	6	5.774	13.54		[+] Br_2 [+]
6	6	5.774	7.56		[+] Ag_1 Ag_1 [+]
7	12	5.774	42.56	1	[+] Br_2 Ag_1 [+]
8	6	5.774	13.35	1	[+] Ag_1 [+] Ag_1 [+]
9	6	5.774	2.87		[+] Ag_1 [+] Ag_1 [+]
10	6	5.774	41.53	2	[+] Ag_1 Br_2 Ag_1 [+]
13	48	5.986	4.74		[+] Br_1 Ag_1 [+]

```
Independent points               =      32.695312500
Number of variables              =       9.000000000
Chi-square                       =   10726.708177990
Reduced Chi-square               =     452.693256440
R-factor                         =       0.000101022
Measurement uncertainty (k)      =       0.000082258
Measurement uncertainty (R)      =       0.045440538
Number of data sets              =       2.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot_Ag          =     0.7340500   +/-      4.9613600     (0.0000)
  delr1            =    -0.0200840   +/-      0.0184400     (0.0000)
  ss1              =     0.0016700   +/-      0.0009520     (0.0030)
  enot_Br          =     3.3626850   +/-      0.7024480     (0.0000)
  delr2            =    -0.1797630   +/-      0.0287640     (0.0000)
  ss2              =     0.0008700   +/-      0.0007880     (0.0030)
  delr3            =    -0.0567180   +/-      0.0027450     (0.0000)
  ss3              =     0.0048650   +/-      0.0000780     (0.0030)
  x                =     0.4994110   +/-      0.2164290     (0.5000)

Set parameters:
  amp              =  0.9
```





Resumo dos resultados do ajuste

Arranjo dos ânions	**Enot**	**r (Å)**			**Sigma^2 (10^{-3})**			**Delta r**			**x**
		Ag-Br	**Ag-Cl**	**Ag-Br**	ss1	ss2	ss3	Delr1	Delr2	Delr3	
Facial	0.73	2.86	2,70	2.83	1.68±0.95	0.83±0.8	4.8±0.07	-0.02±0.018	-0.18±0.029	-0.056±0.07	0.49±0.21
Meridiano	0.73	2.86	2.70	2.83	1.67±0.95	0.87±0.78	4.8±0.07	-0.02±0.018	-0.17±0.028	-0.056±0.002	0.49±0.21