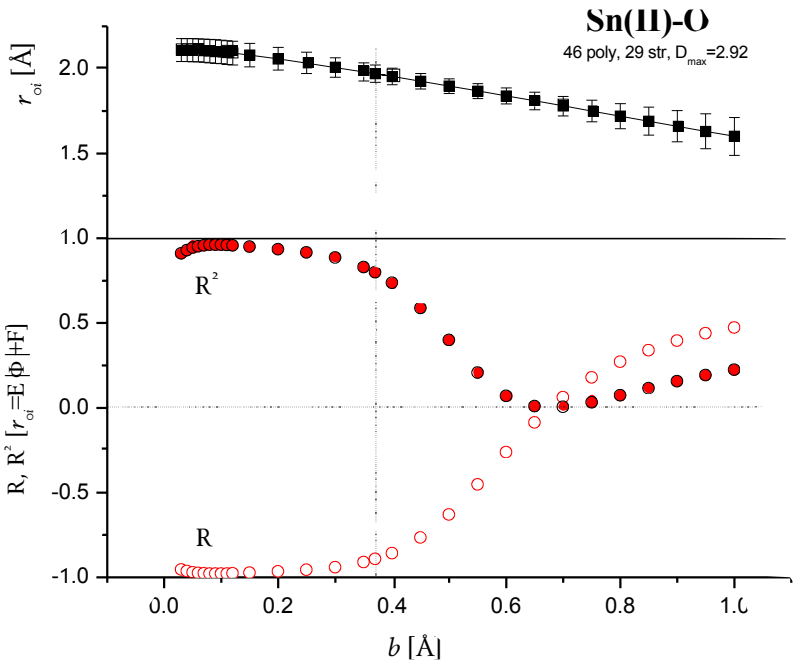
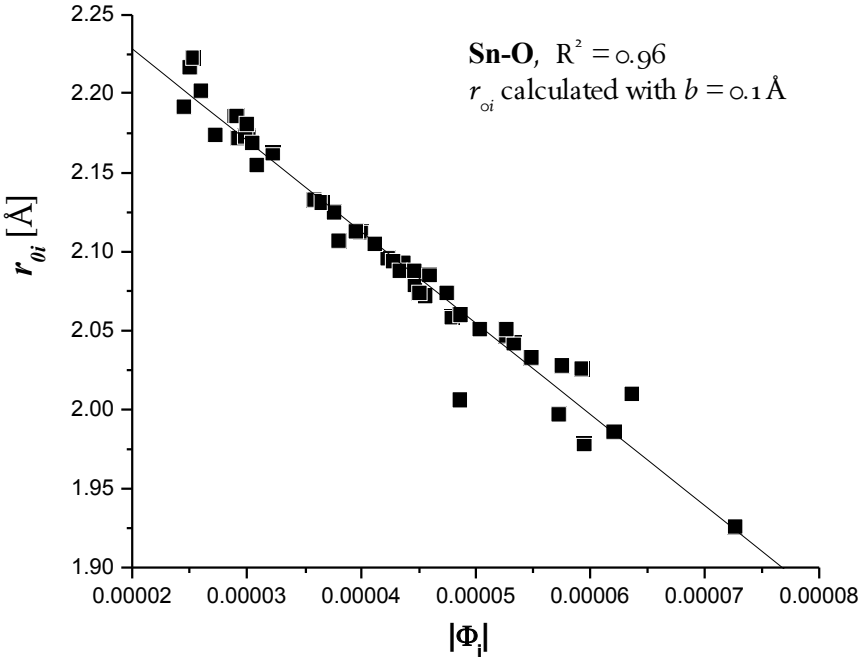
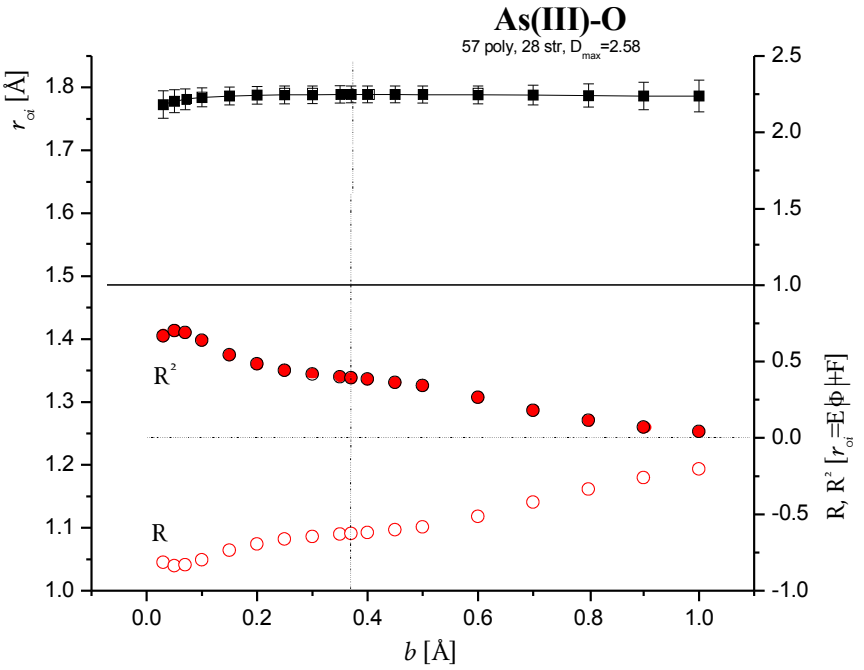
Supplementary material for sn5045

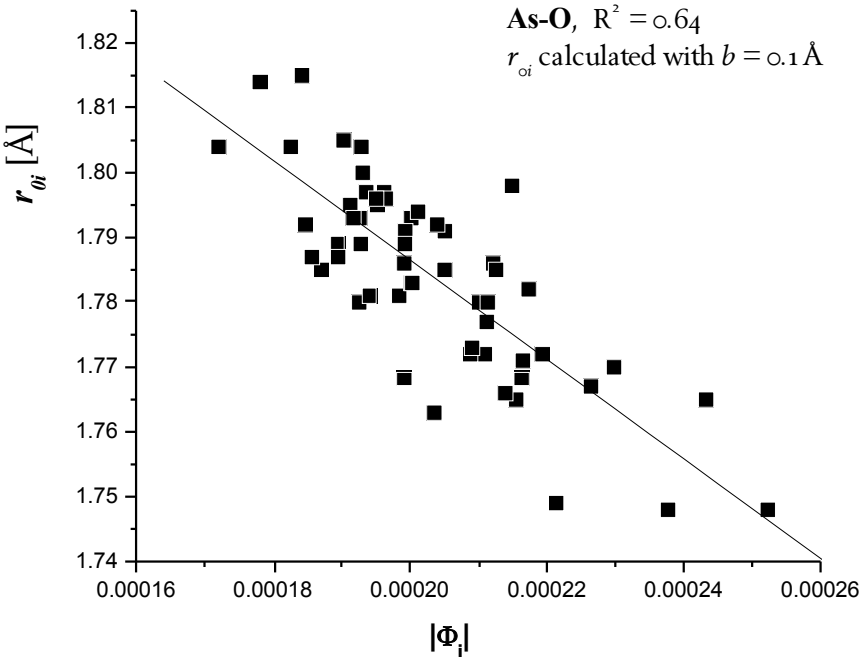
Influence of variation of b on correlations r_{oi} *versus* $|\mathbf{\Phi}_i|$

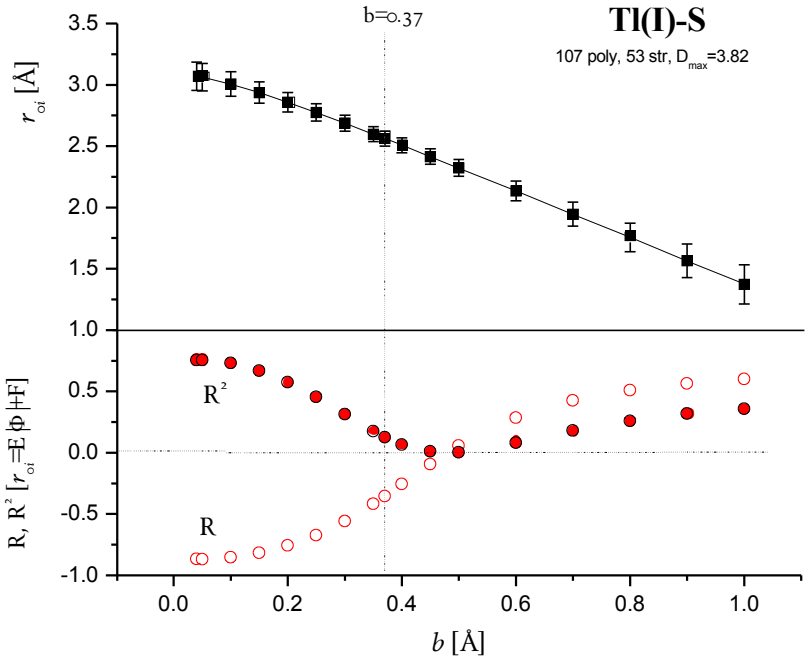
To study this influence, three data sets of [$\mathbf{LX}_n$] polyhedra have been selected: [$Sn^{II}O_n$] with good, [$As^{III}O_n$] with moderate and [$Tl^{I}S_n$] with poor fit of r_{oi} values (calculated with b = 0.37Å) *versus* $|\mathbf{\Phi}_i|$. For each of these data sets, the mean value of r_{oi} and its standard deviation were calculated as a function of b. Subsequently, the correlation coefficients R and R^2 were calculated for $r_{oi} = E\ |\Phi_i| + F$ for the given b value. In each diagram, the mean value and standard deviation (as error bar) of r_{oi} and the R, R^2 values are plotted against b.

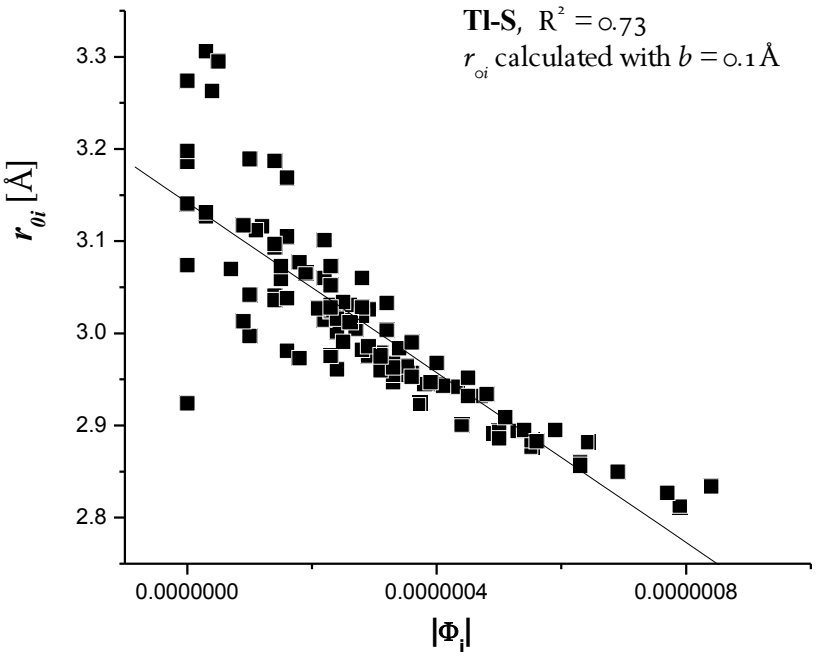

Sn(II)-O
46 poly, 29 str, D_max=2.92
r_oi [Å]
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
R²
R
R, R² [r_oi=E|Φ|+F]
0.0
0.2
0.4
0.6
0.8
1.0
b [Å]


Sn-O, R² = 0.96
r_oi calculated with b = 0.1 Å
r_0i [Å]
2.25
2.20
2.15
2.10
2.05
2.00
1.95
1.90
0.00002
0.00003
0.00004
0.00005
0.00006
0.00007
0.00008
|Φ_i|


As(III)-O
57 poly, 28 str, D_max=2.58
r_oi [Å]
R, R² [r_oi=E|Φ|+F]
R²
R
b [Å]


As-O, R² = 0.64
r_oi calculated with b = 0.1 Å
r_0i [Å]
|Φ_i|


b=0.37
Tl(I)-S
107 poly, 53 str, D_max=3.82
r_oi [Å]
R, R² [r_oi=E|Φ|+F]
R²
R
b [Å]


Tl-S, R² = 0.73
r_oi calculated with b = 0.1 Å
r_0i [Å]
|Φ_i|