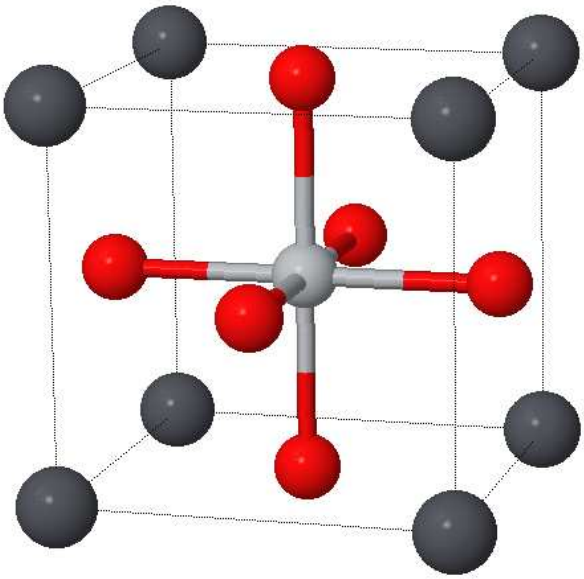
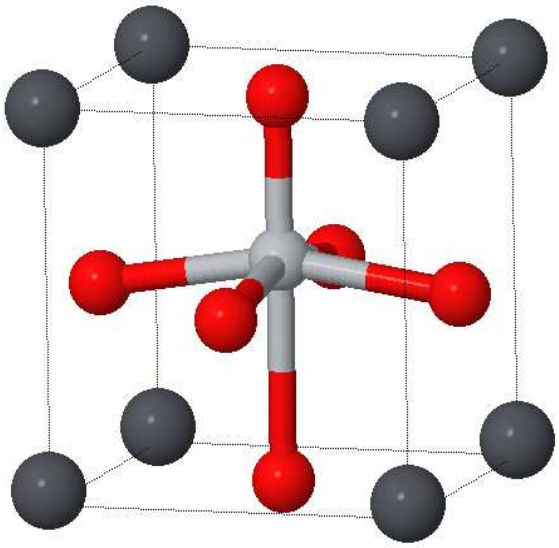
EXAFS analysis of distorted metal-oxygen octahedra

Anatoly Frenkel (Yeshiva University) and Joshua Kas (University of Washington)

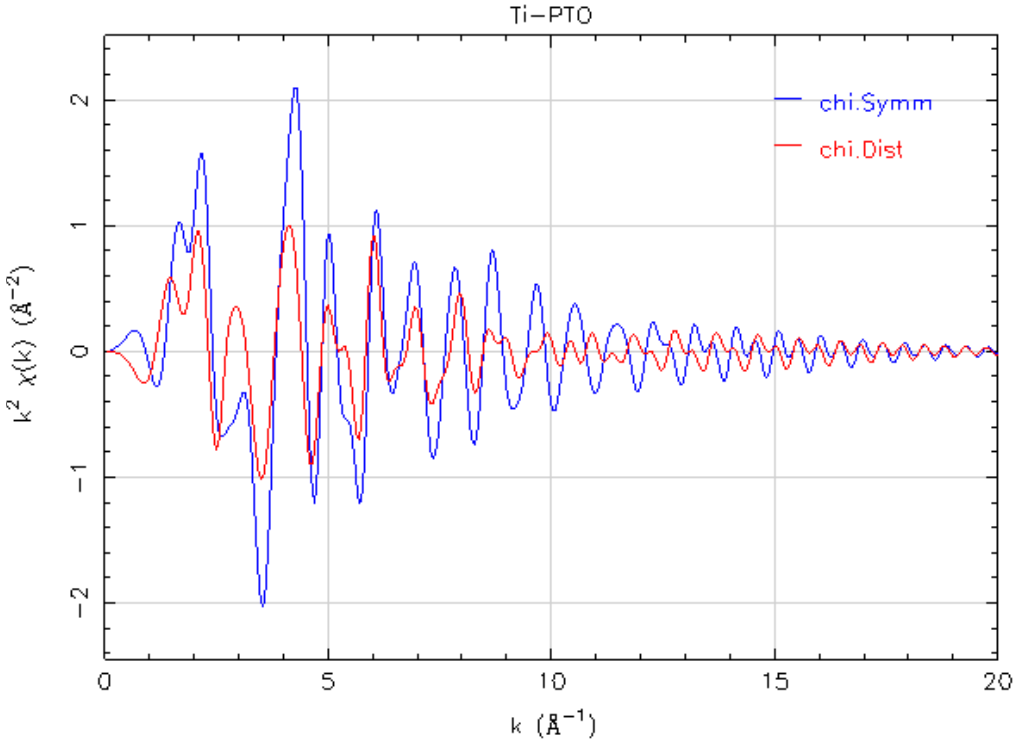


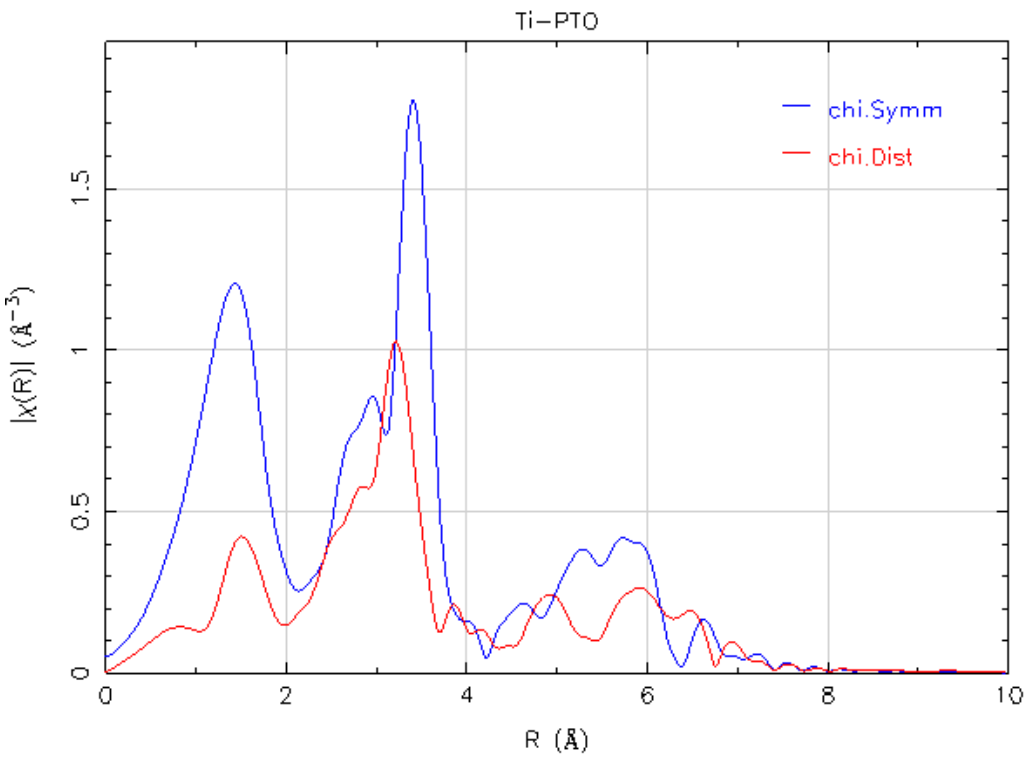
Undistorted $PbTiO_3$



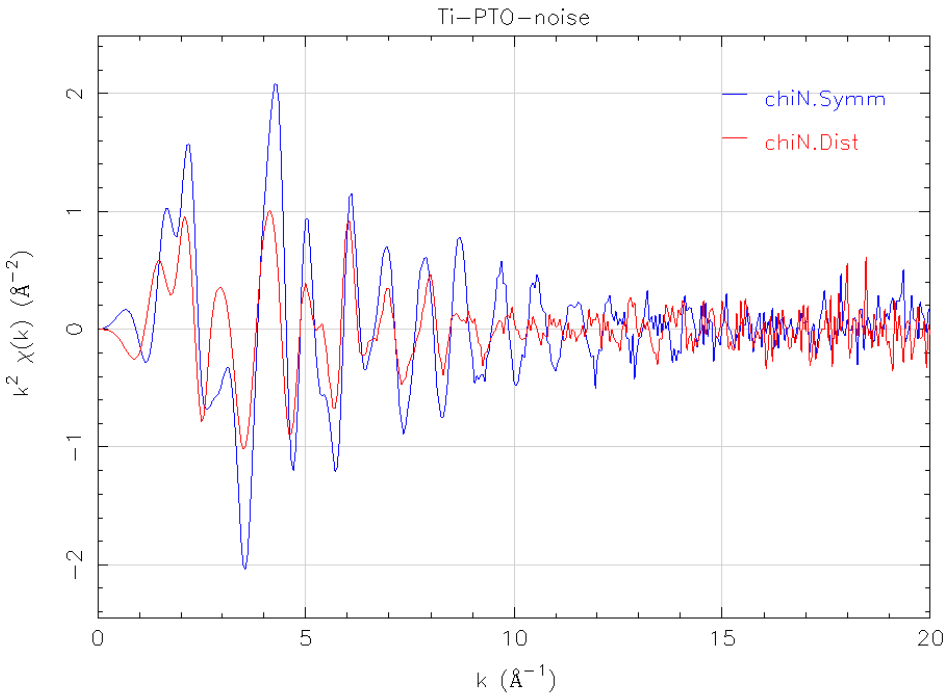
Distorted $PbTiO_3$

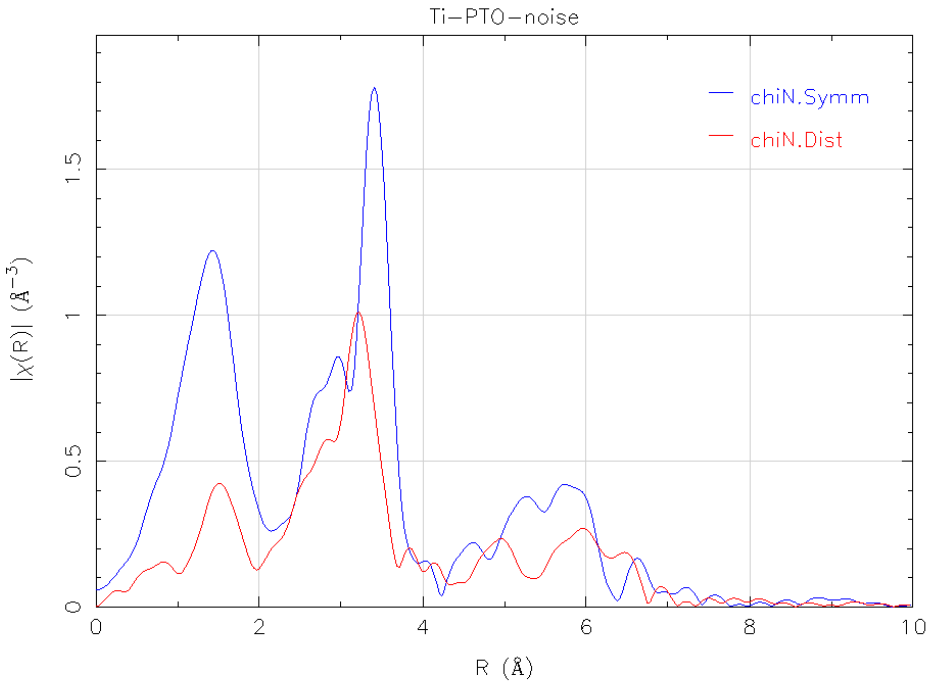
Without noise:





With noise added:





1. Fitting "symmetric data" with centrosymmetric model (up to the 3rd shell)

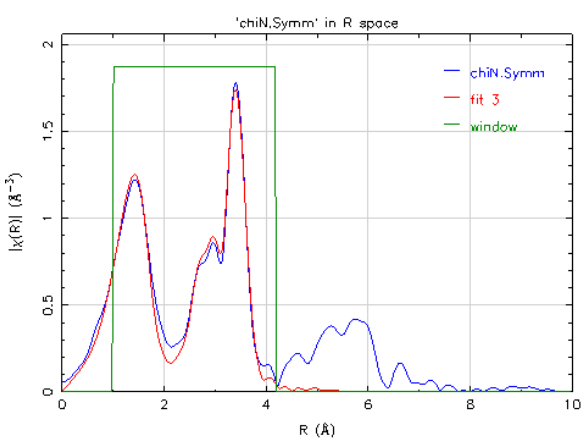
Independent points = 22.028320312
Number of variables = 6.000000000
Chi-square = 445.605384863
Reduced Chi-square = 27.801128014
R-factor = 0.008673927
Measurement uncertainty (k) = 0.000509626
Measurement uncertainty (R) = 0.012387999
Number of data sets = 1.000000000

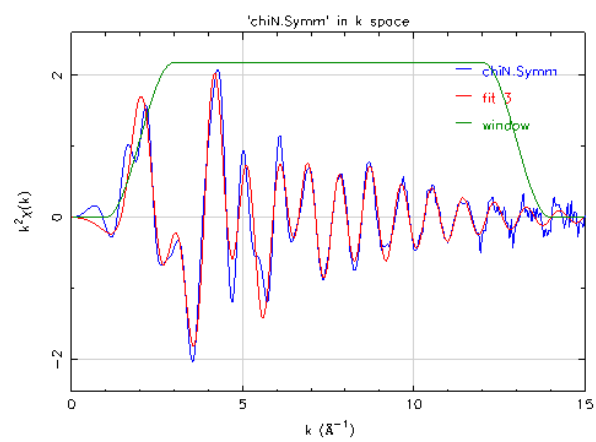
Guess parameters +/- uncertainties (initial guess):

enot	=	-4.6295660	+/-	0.3506410	(0.0000)
eps	=	-0.0013600	+/-	0.0012100	(0.0000)
ssO1	=	0.0156650	+/-	0.0007640	(0.0050)
ssPb	=	0.0085830	+/-	0.0006070	(0.0050)
ssTi	=	0.0118630	+/-	0.0005630	(0.0050)
ss3	=	0.0409810	+/-	0.0185680	(0.0050)

Verifiable information:

R(Ti-O) = 1.997(2) Å
ssO1 = 0.0157(8) Å^2
ssPb = 0.0086(6) Å^2
ssTi = 0.0119(6) Å^2





2. Fitting the centrosymmetric data with symmetric model: 1st shell only (k, k2, k3 weighting)

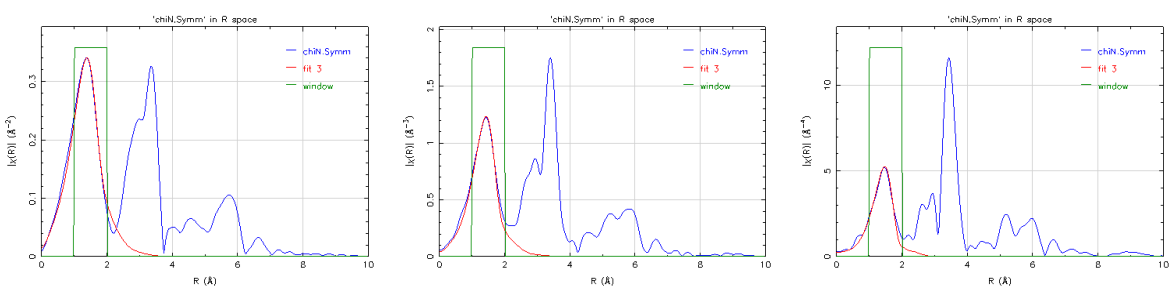
Independent points = 6.468750000
Number of variables = 3.000000000
Chi-square = 605.668418646
Reduced Chi-square = 174.607111682
R-factor = 0.005584699
Measurement uncertainty (k) = 0.000498354
Measurement uncertainty (R) = 0.001124370
Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):

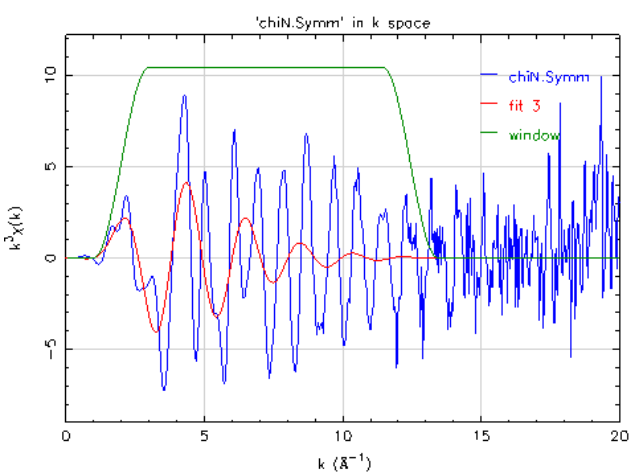
enot	=	-4.8710440	+/-	0.8746870	(0.0000)
do1	=	0.0036570	+/-	0.0113700	(0.0000)
ssO1	=	0.0163850	+/-	0.0008250	(0.0050)

Def parameters (using "FEFF0: Path 1: [O_1]"):

S02	=	1.0000000
N	=	6.0000000



Comment on the k-range in the fit:



3. Fitting "distorted" data with the 001 displacement model (k, k2, k3 weighting)

Independent points = 5.479492188
Number of variables = 4.000000000
Chi-square = 922.889365348
Reduced Chi-square = 623.787927470
R-factor = 0.060700397
Measurement uncertainty (k) = 0.000473843
Measurement uncertainty (R) = 0.000904154
Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):

enot	**=**	**-6.0255970**	**+/-**	**5.4047610**	**(-5.1500)**
ssO1	**=**	**0.0200670**	**+/-**	**0.0052720**	**(0.0050)**
dr_1	**=**	**-0.3348410**	**+/-**	**0.0507450**	**(-0.1000)**
dr_2	**=**	**0.0223810**	**+/-**	**0.0390490**	**(0.0000)**

Def parameters (using "FEFF0: Path 1: [O_1]"):

S02	=	1.0000000
ssO2	=	0.0200670
ssO3	=	0.0200670

Verifiable information:

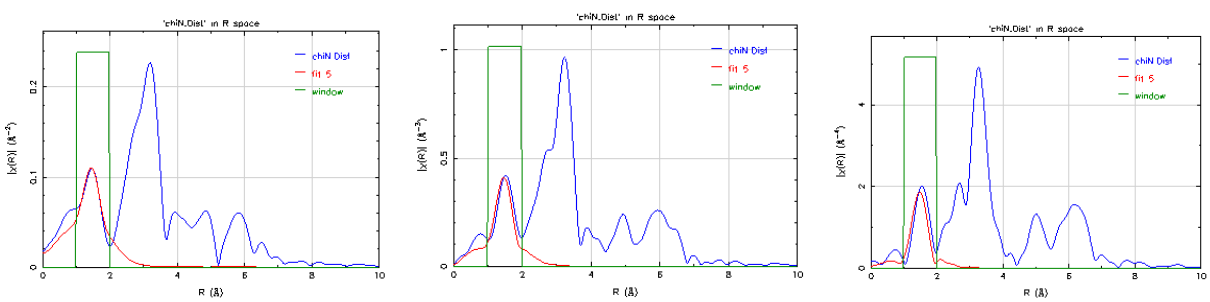
R(Ti-O1): 1.67(5) Å

R(Ti-O2): 2.02(4) Å

R(Ti-O3): 2.33(5) Å

ssO1: 0.020(5) Å^2

K_{max}= 11 **Å**$^{-1}$. Spatial resolution criterion: $\Delta r = \dfrac{\pi}{2k_{\max}}$ =0.13 **Å, so this result is meaningful.**



4) Fitting symmetric data with distorted model:

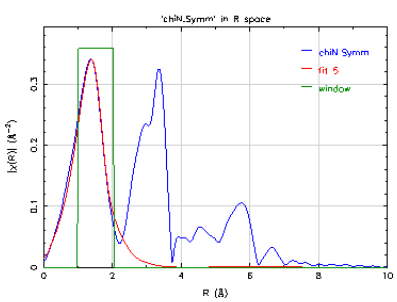
Independent points = 6.413085937
Number of variables = 4.000000000
Chi-square = 819.290141518
Reduced Chi-square = 339.519670139
R-factor = 0.005439781
Measurement uncertainty (k) = 0.000489350
Measurement uncertainty (R) = 0.001051684
Number of data sets = 1.000000000

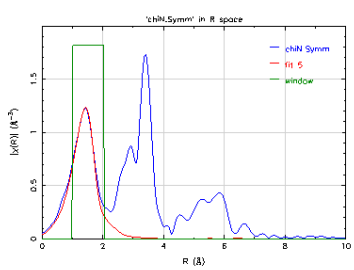
Guess parameters +/- uncertainties (initial guess):

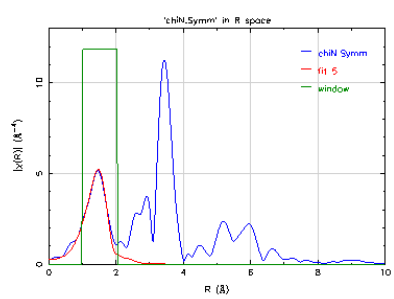
enot	**=**	**-4.8494440**	**+/-**	**1.6993360**	**(-5.1500)**
ssO1	**=**	**0.0137820**	**+/-**	**0.0684790**	**(0.0000)**
dr_1	**=**	**-0.0890930**	**+/-**	**1.1592810**	**(-0.1000)**
dr_2	**=**	**0.0052630**	**+/-**	**0.0414460**	**(0.0000)**

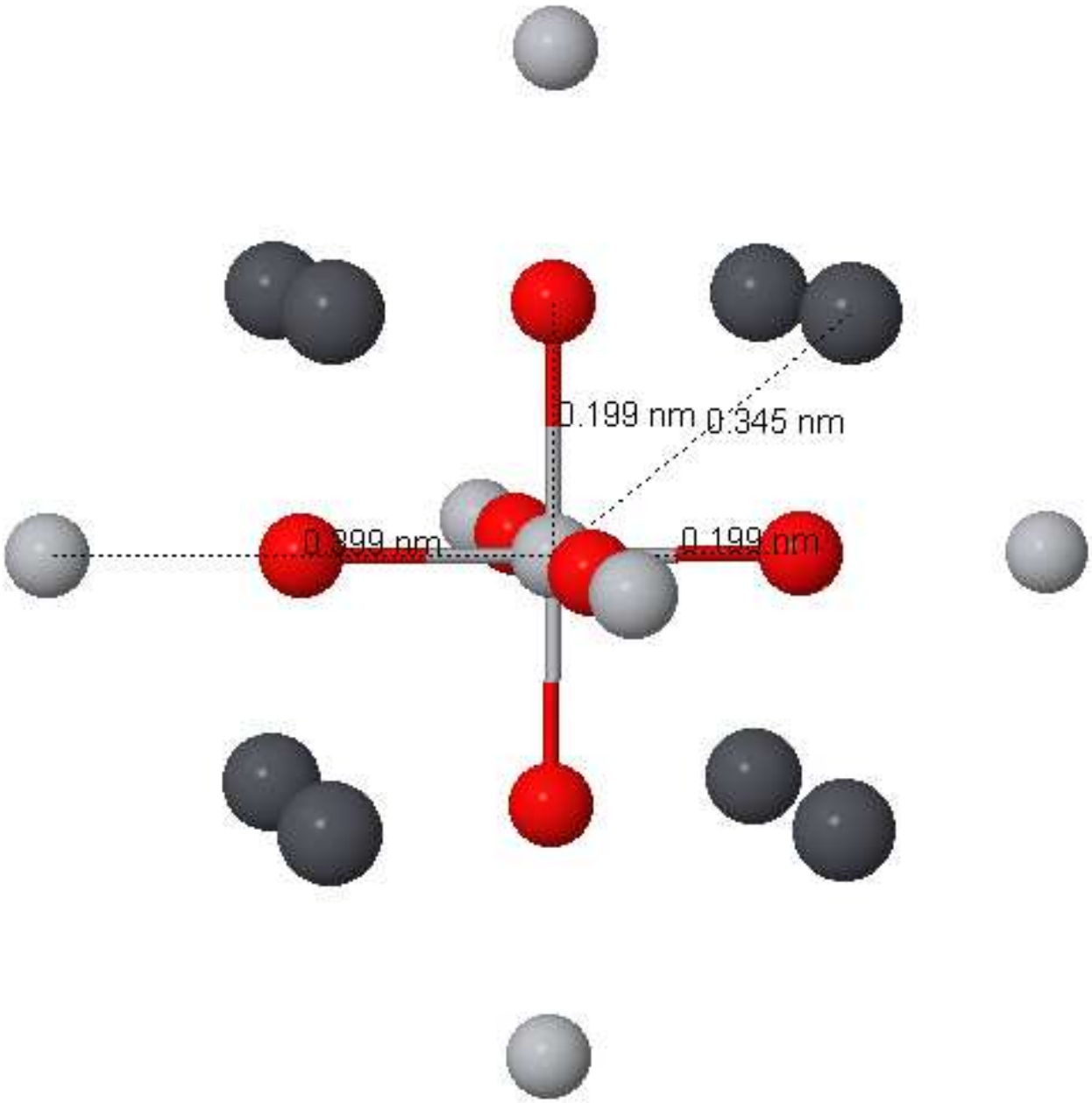
Def parameters (using "FEFF0: Path 1: [O_1]"):

S02 = 1.0000000
ssO2 = 0.0137820
ssO3 = 0.0137820







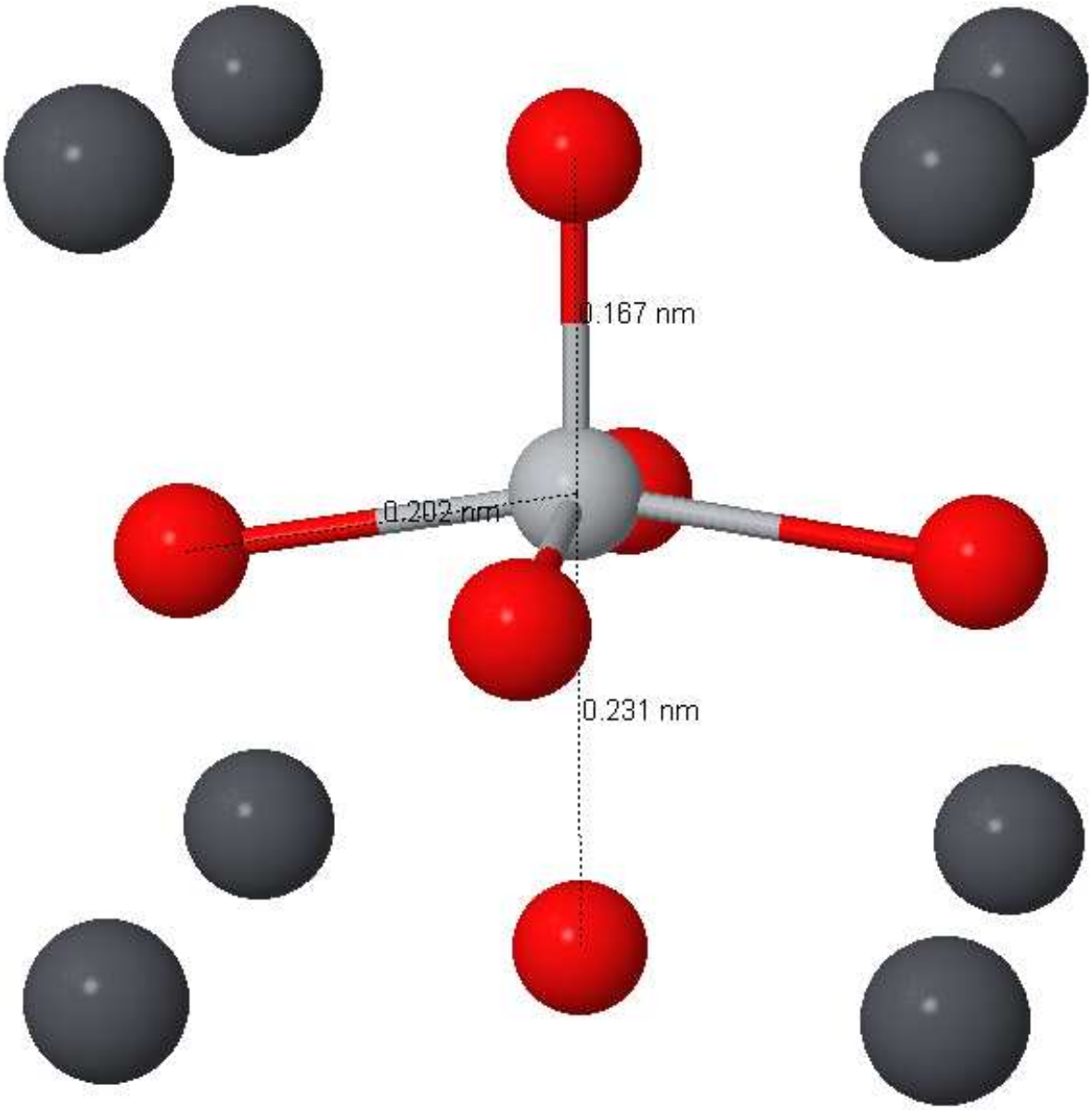


Input:

ssO1 = 0.0186 Å^2

Output of the analysis:

R(Ti-O1): 2.00(1) Å
ssO1: 0.0164(8) Å^2



Input:

ssO1 = 0.0159 Å^2
ssO2 = 0.0192 Å^2
ssO3 = 0.0217 Å^2

Output of the analysis:

R(Ti-O1): 1.67(5) Å
R(Ti-O2): 2.02(4) Å
R(Ti-O3): 2.33(5) Å

ssO1=ssO2=ssO3: 0.020(5) Å^2