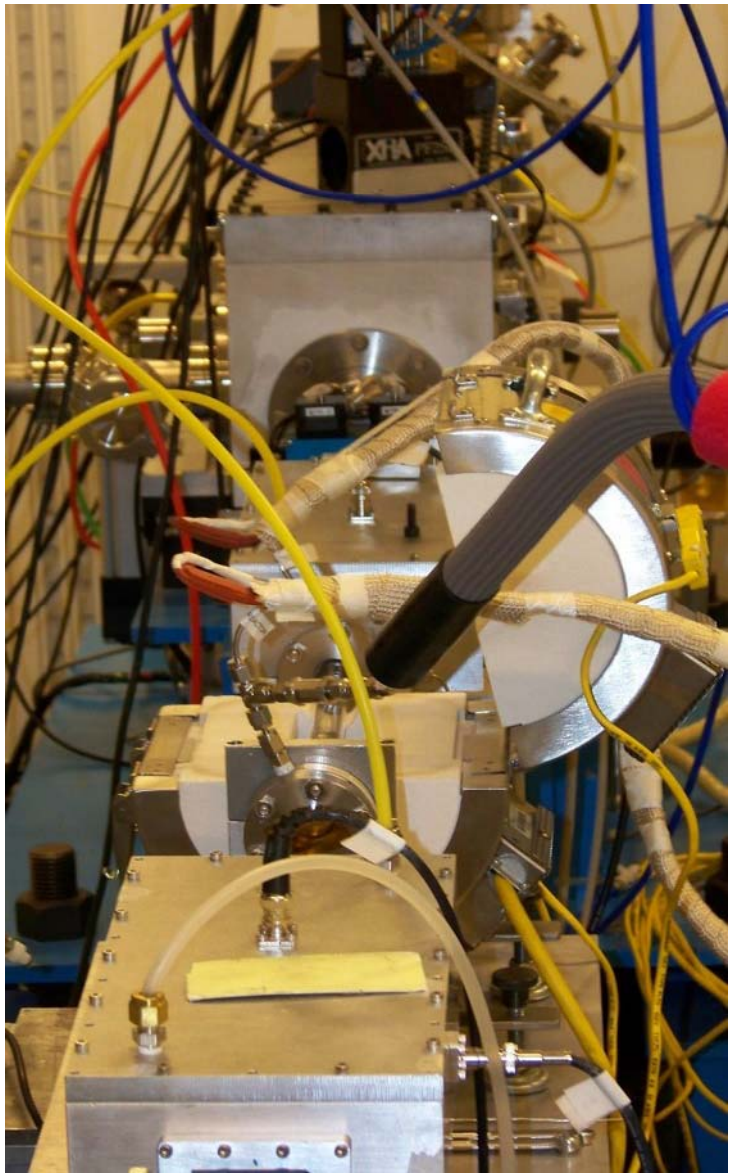

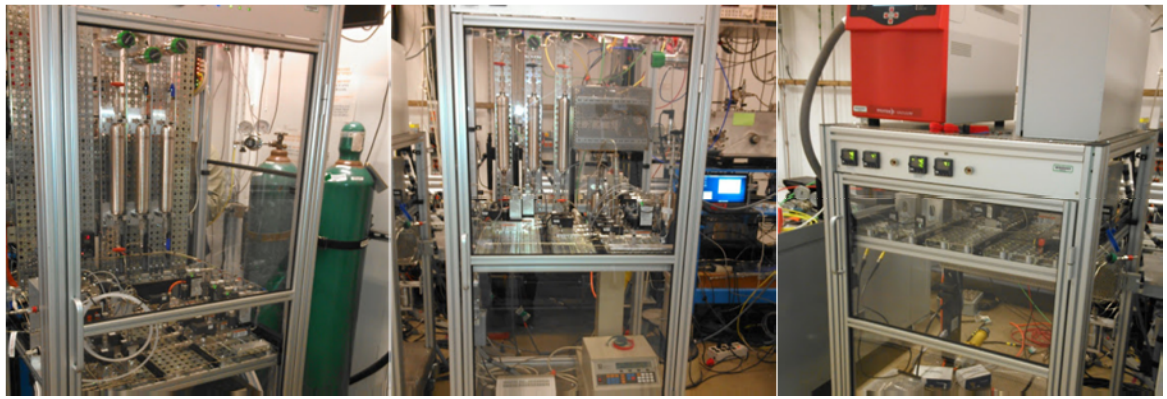

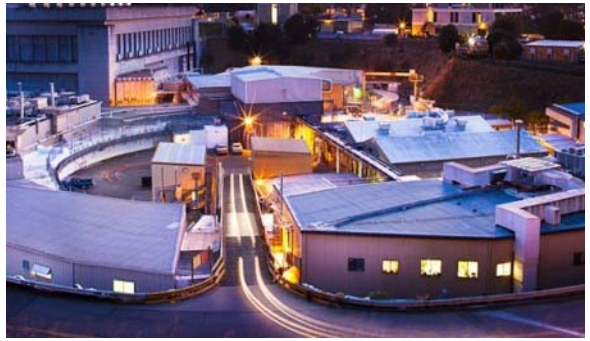

Shelly D. Kelly

Nov. 3, 2016

MULTIPLE SCATTERING PATHS

NSLSII EXAFS Workshop

Honeywell UOP

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Outline

- Uranyl XANES
- Multiple scattering paths
- Parameterization multiple scattering paths
- Example of data analysis with and without MS
- Other examples of multiple scattering paths.

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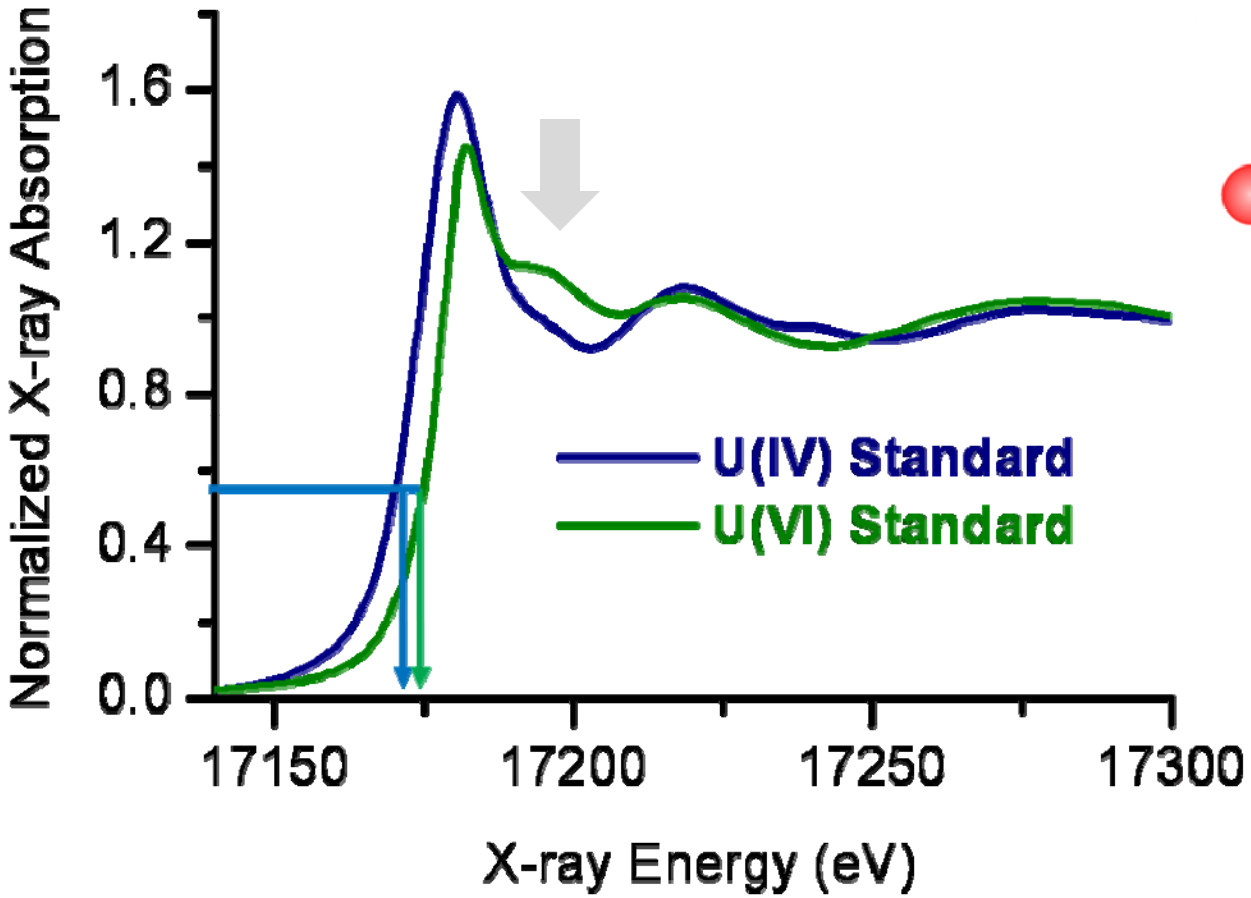
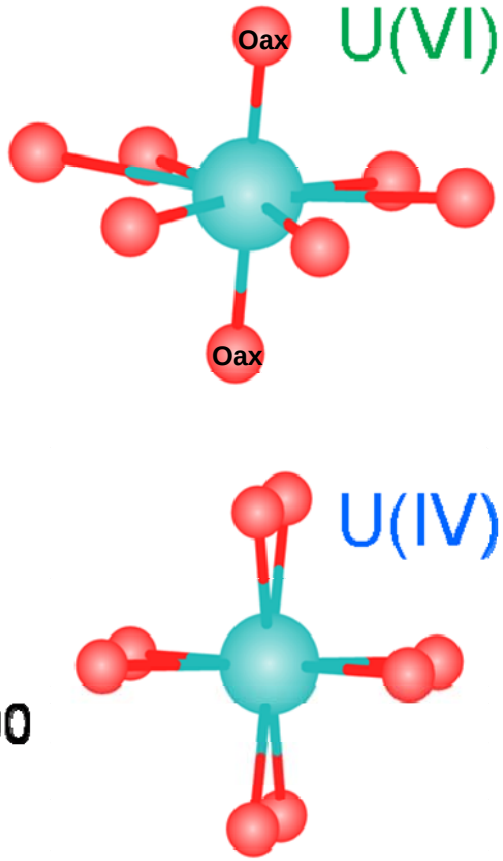
Uranium(IV) and Uranium(VI)





- Two tightly bounded axial oxygen atoms from U(VI) contribute to strong multiple scattering.
- Resonance feature above absorption edge is due to multiple scattering from Oax

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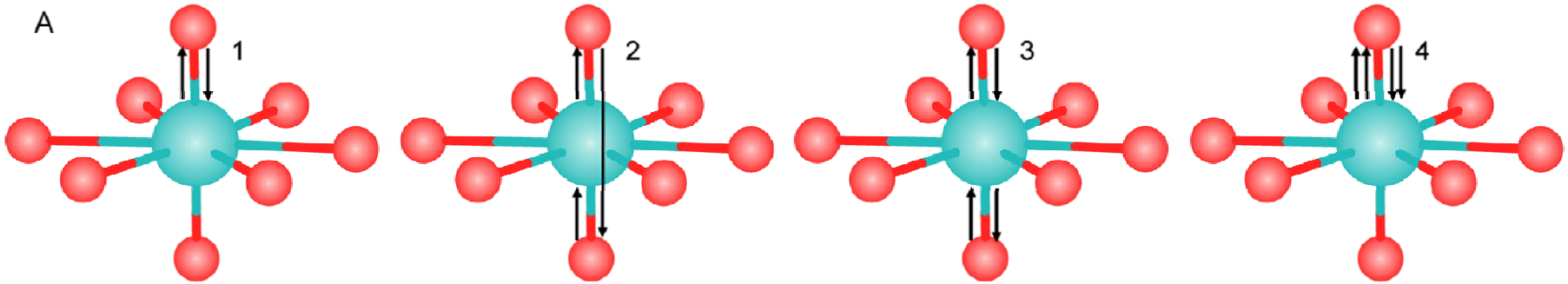
Uranyl Single and Multiple Scattering Paths



2 leg	3 leg	4 leg	4 leg (Rattle)
Single Scattering	Multiple Scattering	Multiple Scattering	Multiple Scattering

- Distances and sigma2 terms are not independent for these paths.

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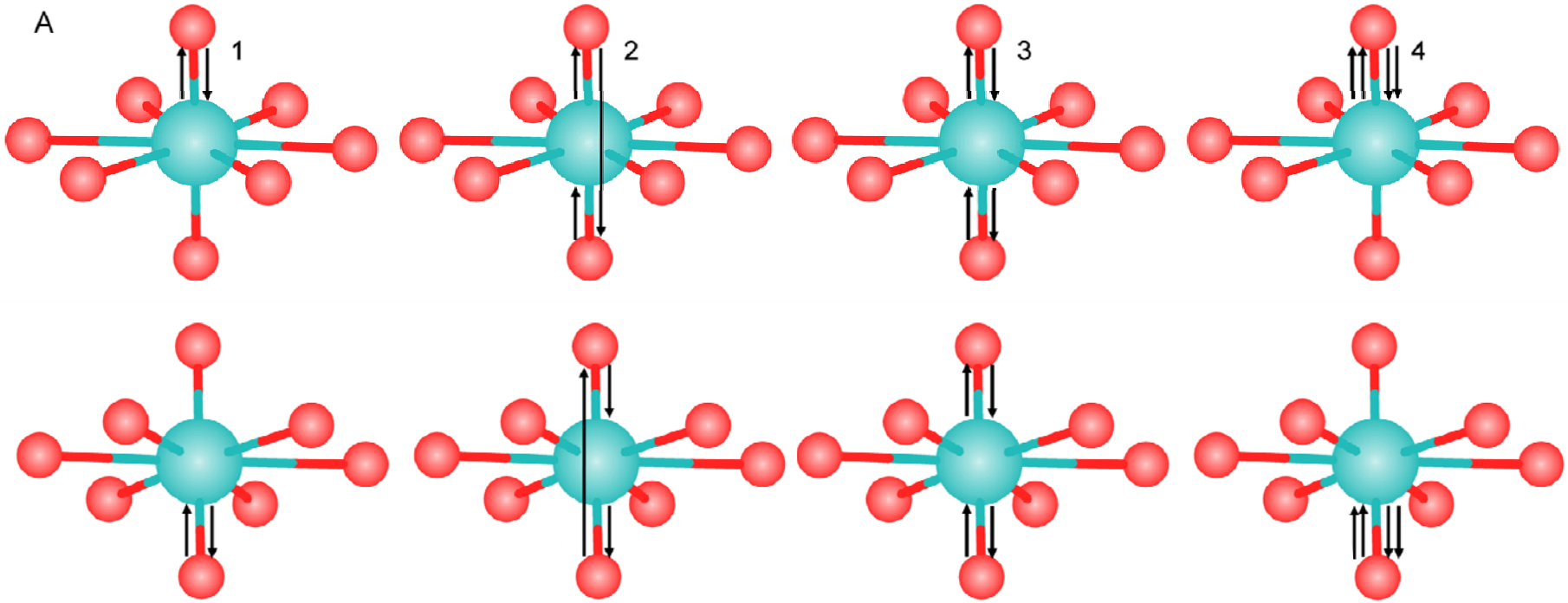
Coordination Number (Degeneracy)



2 leg	3 leg	4 leg	4 leg (Rattle)
Single Scattering	Multiple Scattering	Multiple Scattering	Multiple Scattering

- Number of equivalent paths is 2 for each configuration

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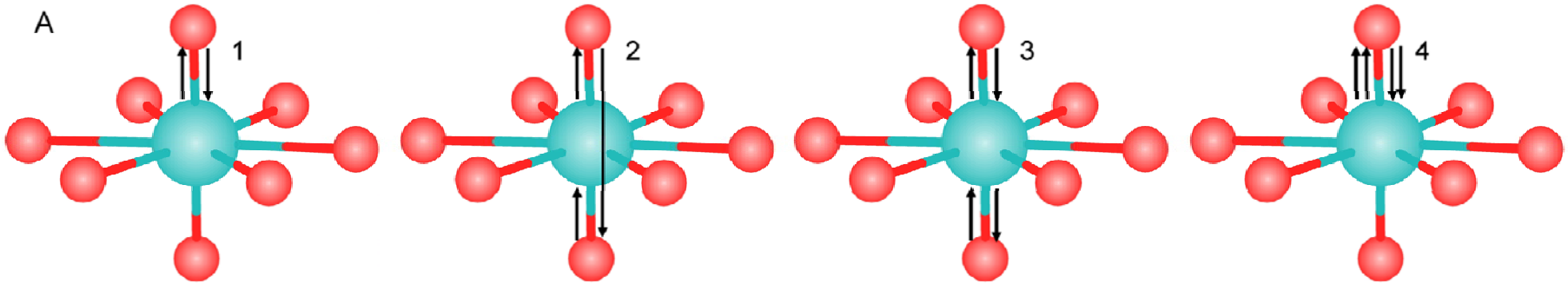
Mean square displacement



2 leg Single Scattering	3 leg Multiple Scattering	4 leg Multiple Scattering	4 leg (Rattle) Multiple Scattering
σ^2	$\sim 2x\ \sigma^2$	$\sim 2x\ \sigma^2$	$4x\ \sigma^2$

$$\left\langle \left(\vec{r}_i - \vec{r}_o \right)^2 \right\rangle_i \equiv \sigma^2$$

Instantaneous position

Equilibrium position

- σ^2 terms are not independent for these paths.

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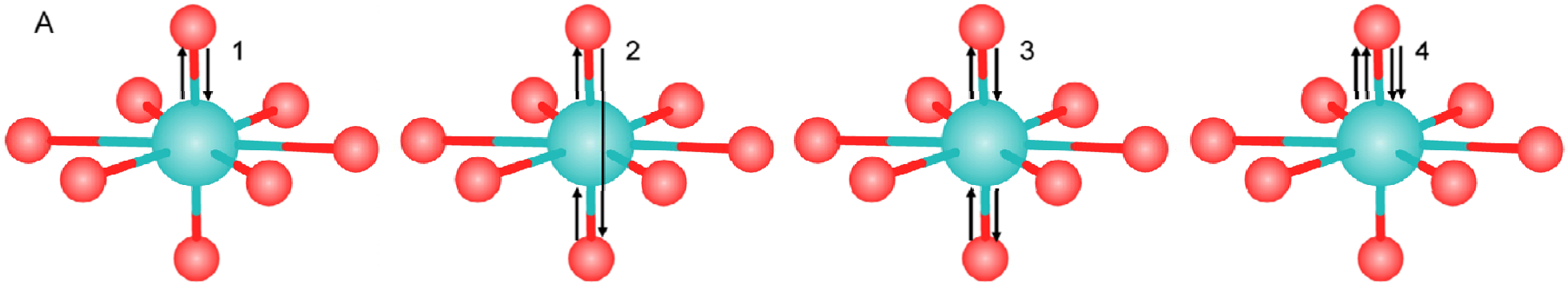
Uranyl Single and Multiple Scattering Paths



2 leg
Single Scattering

3 leg
Multiple Scattering

4 leg
Multiple Scattering

4 leg (Rattle)
Multiple Scattering

Parameter	2 leg SS	3 leg MS	4 leg MS	4 leg MS (Rattle)
CN	2	2	2	2
R	R_{Oax}	2x R_{Oax}	2x R_{Oax}	2x R_{Oax}
σ^2	σ^2	~2x σ^2	~2x σ^2	4x σ^2

- Single R and σ^2 can be used to parameterize all 4 paths.

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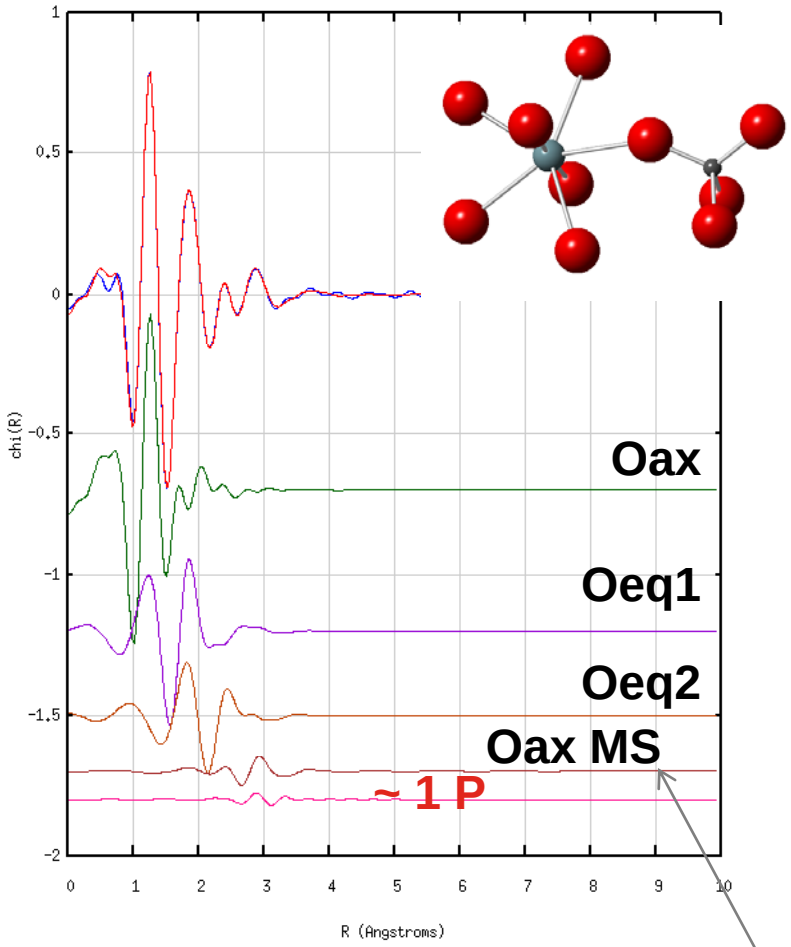
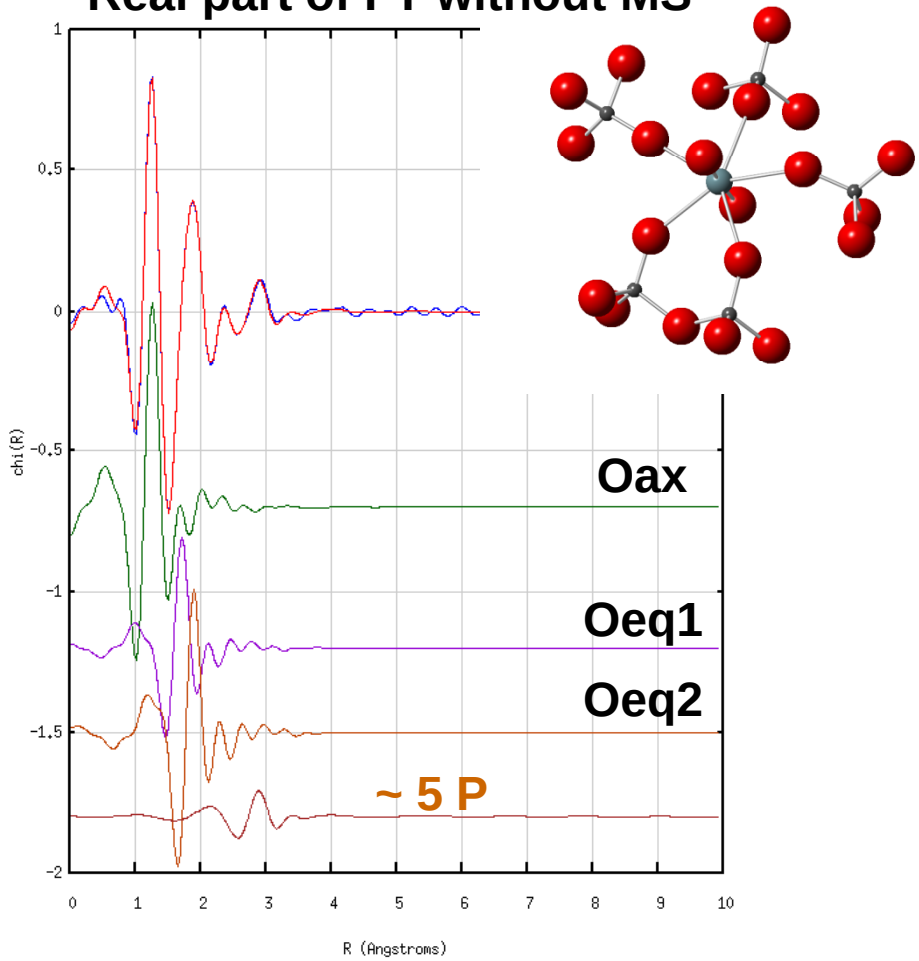
Model Results with and without MS

Real part of FT with MS



Real part of FT without MS



- Best practice to combine 3 MS paths into a single path.
- Number of P neighbors changes from less than 1 to more than 5

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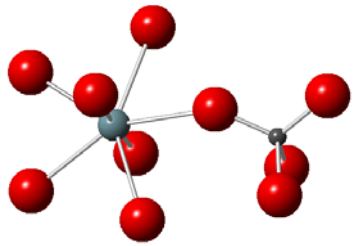
Model Results with and without MS

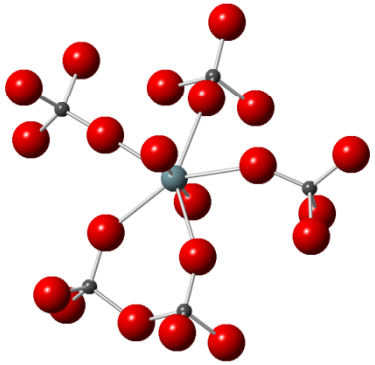
Model results with MS



r-factor = 0.05%

Reduced chi-square 16

Model results without MS



r-factor = 0.1%

Reduced chi-square 36

2x 16 < 36

- Model without MS is statistically not as good as compared to model with MS. Reduced chi-squared increase by more than 2x without MS compared to with MS
- Need to use knowledge of system to also guide selection of the best model.

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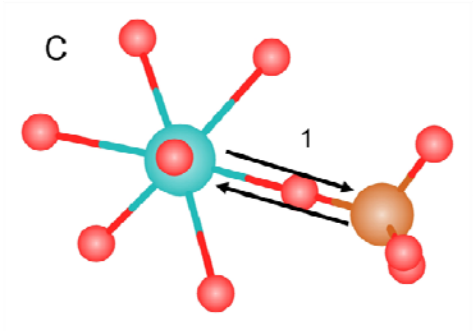
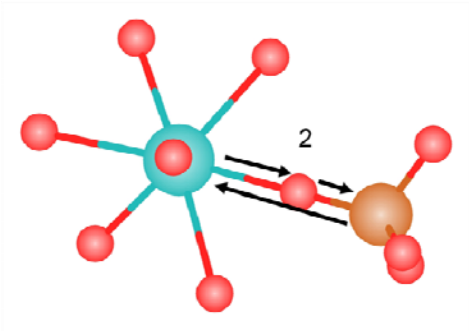
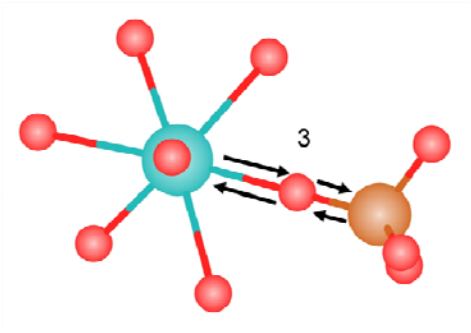
Uranyl Phosphate Single and Multiple Scattering Paths

Uranyl Phosphate







Parameter	2 leg SS	3 leg MS	4 leg MS
CN	1	2	1
R	R_p	$\sim R_p$	$\sim R_p$
σ^2	σ^2	$\sim\sigma^2$	$\sim\sigma^2$

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