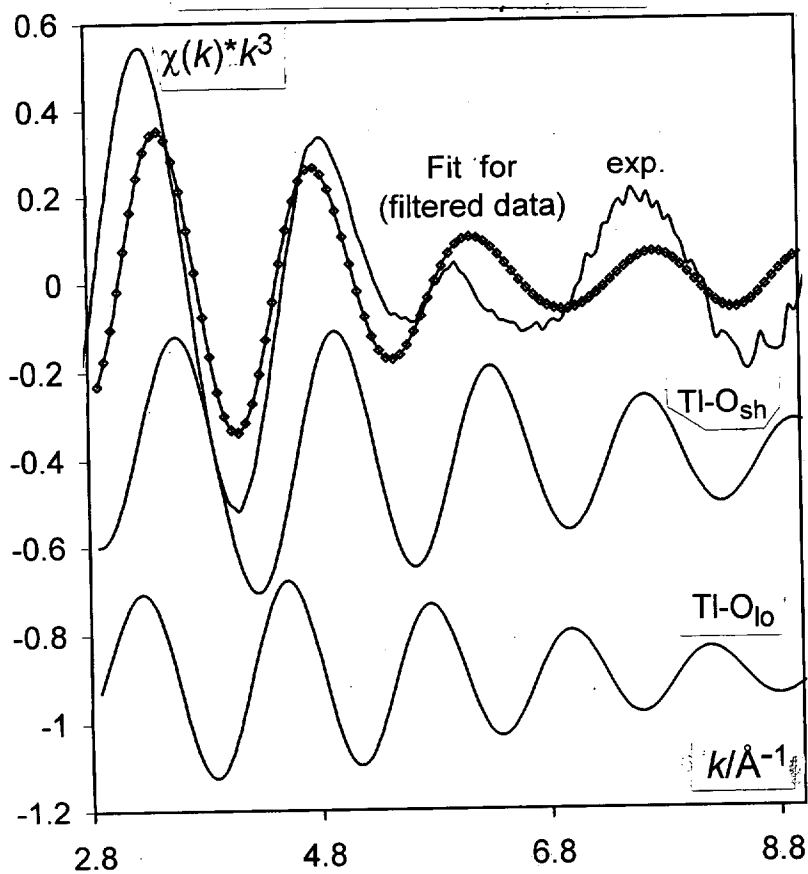


### Supporting Material

*Fig. S1.* Experimental EXAFS and fit (upper) and FT-back-transformed data and fit (lower) in (a)  $k$ -space and (b)  $r$ -space of the hydrated thallium(I) ion in aqueous solution.

*Fig. S2.* Experimental EXAFS and fit (upper) and FT-back-transformed data and fit (lower) in (a)  $k$ -space and (b)  $r$ -space of the  $N,N$ -dimethylthioformamide solvated thallium(I) ion in  $N,N$ -dimethylthioformamide solution.

**Ti(OH<sub>2</sub>)<sub>4</sub><sup>+</sup> Experimental data  
and fit in k-space**



**Ti(OH<sub>2</sub>)<sub>4</sub><sup>+</sup> FT-back-transformed filtered  
data and fit in k-space**

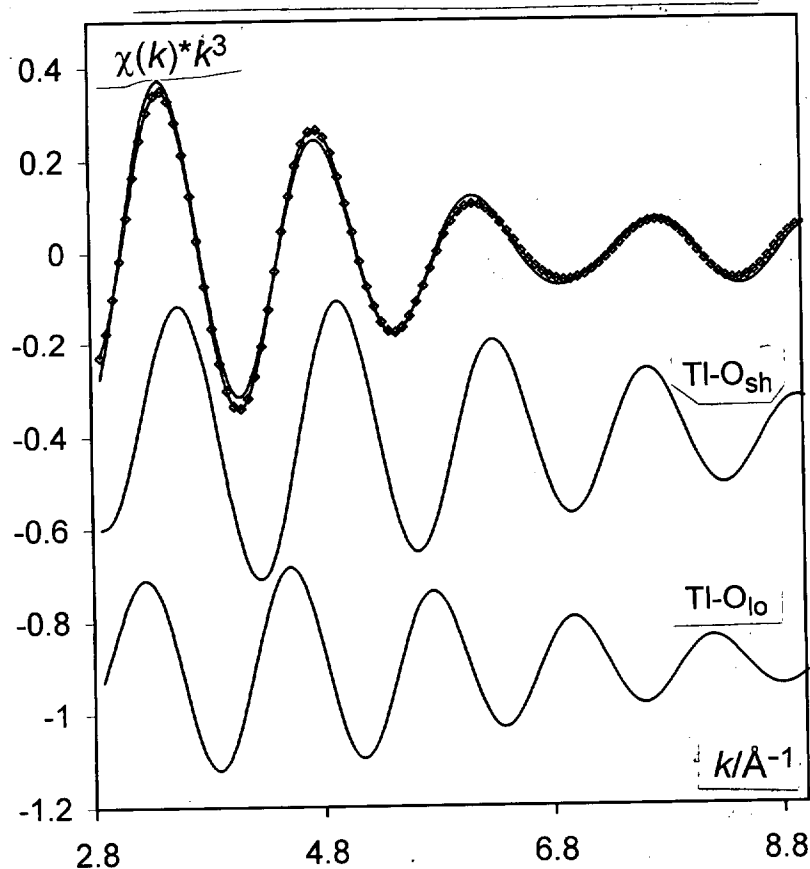
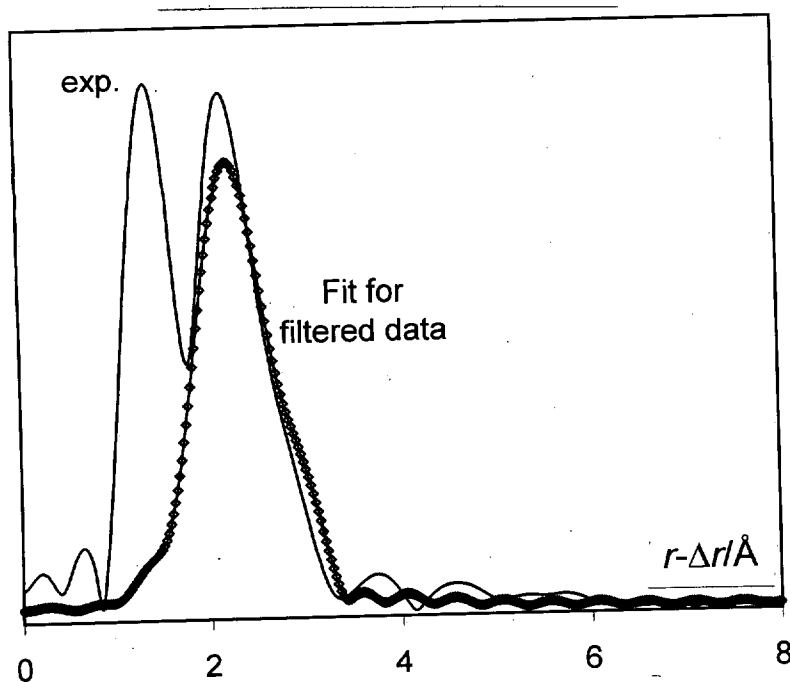


Fig. S70

$\text{Ti}(\text{OH}_2)_4^+$  Experimental data  
and fit in  $r$ -space



$\text{Ti}(\text{OH}_2)_4^+$  FT-back-transformed filtered  
data and fit in  $r$ -space

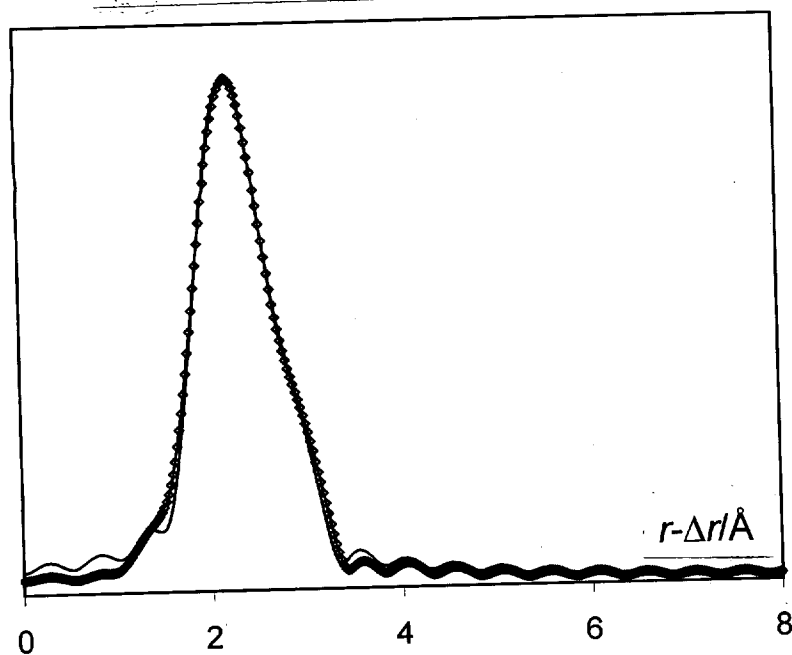
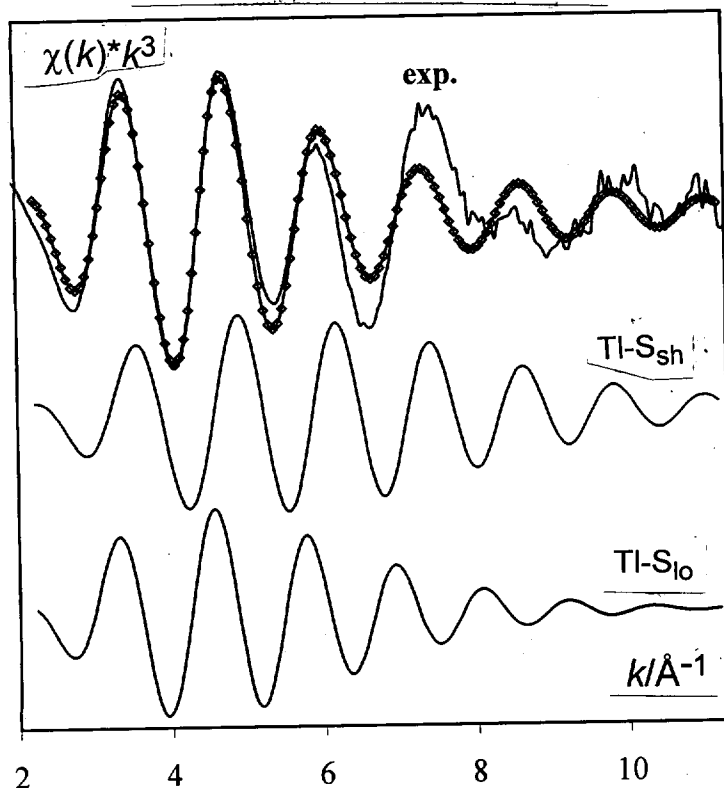
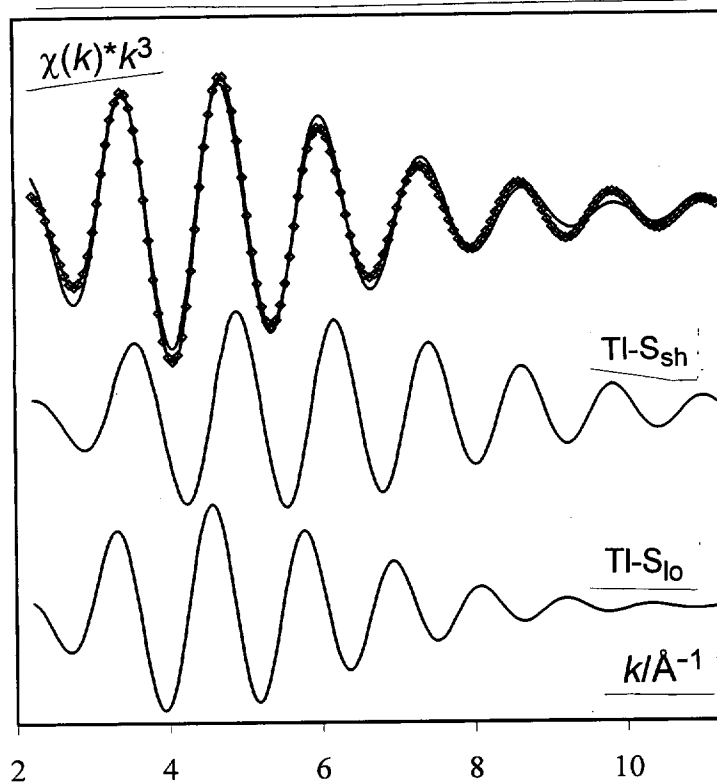


Fig. S2a

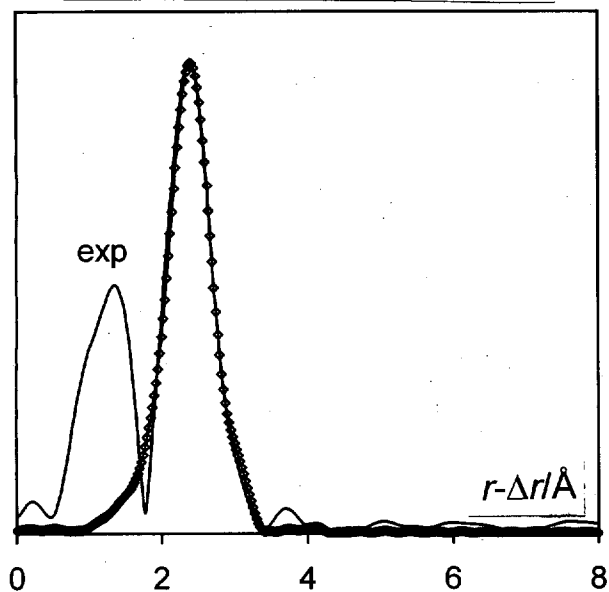
**Tl(dmtf)<sub>6</sub><sup>+</sup> Experimental data  
and fit in k-space**



**Tl(dmtf)<sub>6</sub><sup>+</sup> FT-back-transformed filtered  
data and fit in k-space**



**Tl(dmtf)<sub>6</sub><sup>+</sup> Experimental data  
and fit in *r*-space**



**Tl(dmtf)<sub>6</sub><sup>+</sup> FT-back-transformed filtered  
data and fit in *r*-space**

