Inorganic Chemistry
including bioinorganic chemistry
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Supporting Information.

Figure S1. The XAFS spectra (a) and FT's (b) (modulus and imaginary parts) of Gd^{3+} ion in the aqueous solution: experimental spectra at pH 7.0 and RT (full lines) and MS calculated spectra of the tricapped prism (dashed lines) and square antiprism (dotted line). The first (SS in the first shell), second and third (MS in the first shell) peaks are clearly visible.

Figure S2. The experimental (RT crystal) XAFS spectra (full lines) and MS calculated spectra (dashed lines) of $Gd(DOTA)^-$ complex (a) and $Gd(DTPA)^{2-}$ (b) complexes in the crystals. The first and second shells fitting results also shown (dotted line).

Figure S3. FT's (modulus and imaginary parts) of the experimental (RT crystal) XAFS spectra (full lines) and MS calculated spectra (dashed lines) of $Gd(DOTA)^-$ complex (a) and $Gd(DTPA)^{2-}$ complex (b) in the crystals. The first and second shells fitting results also shown (dotted line).

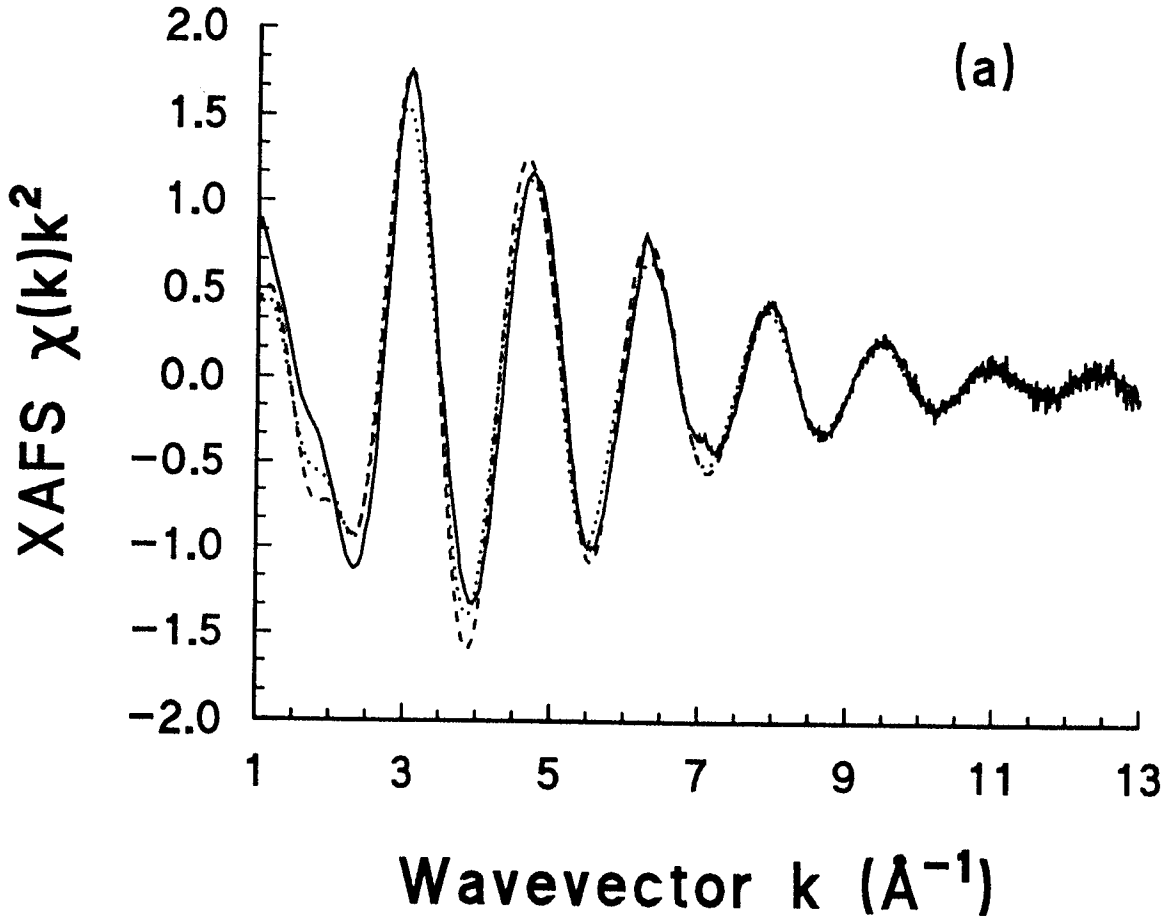

Figure S1a

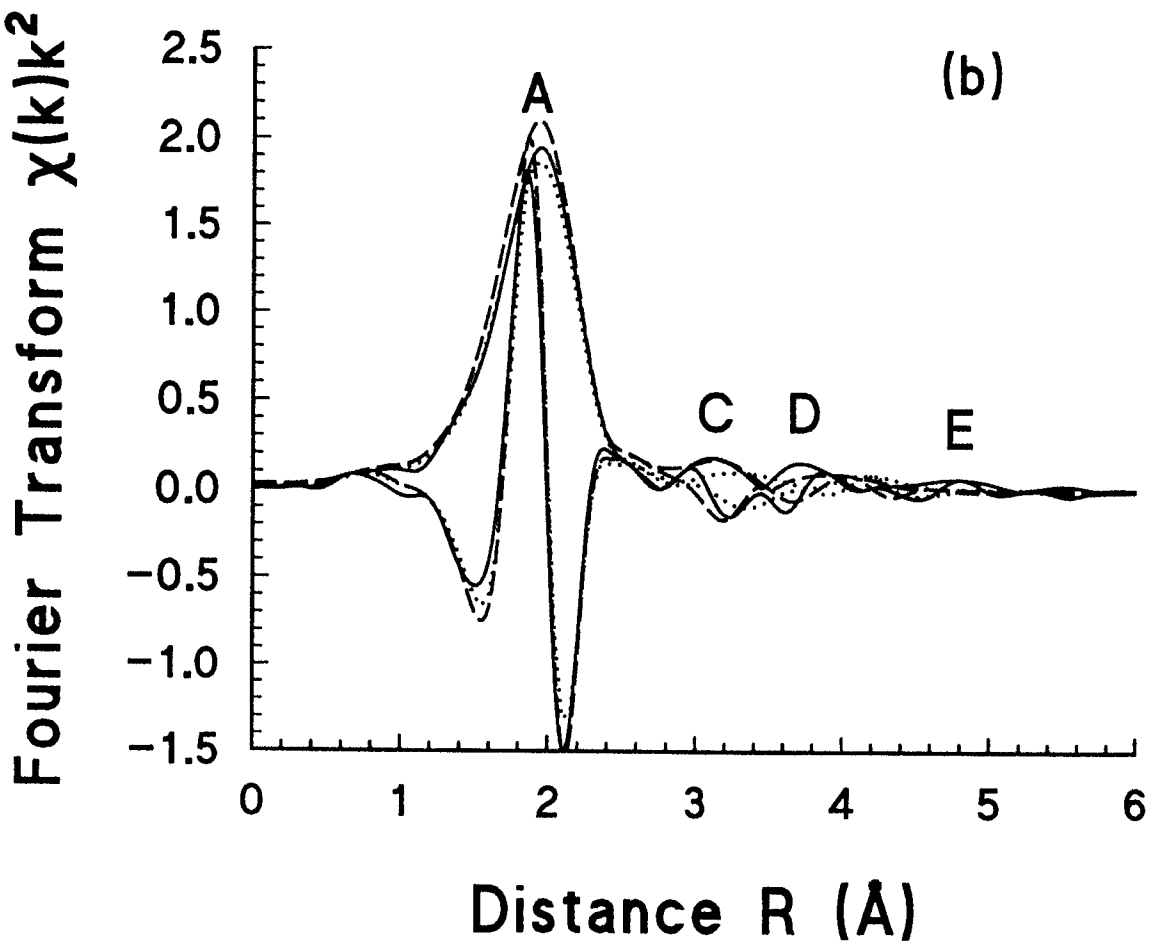
Fourier Transform χ(k)k²
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
1
2
3
4
5
6
A
(b)
C
D
E
Distance R (Å)

Figure S1b

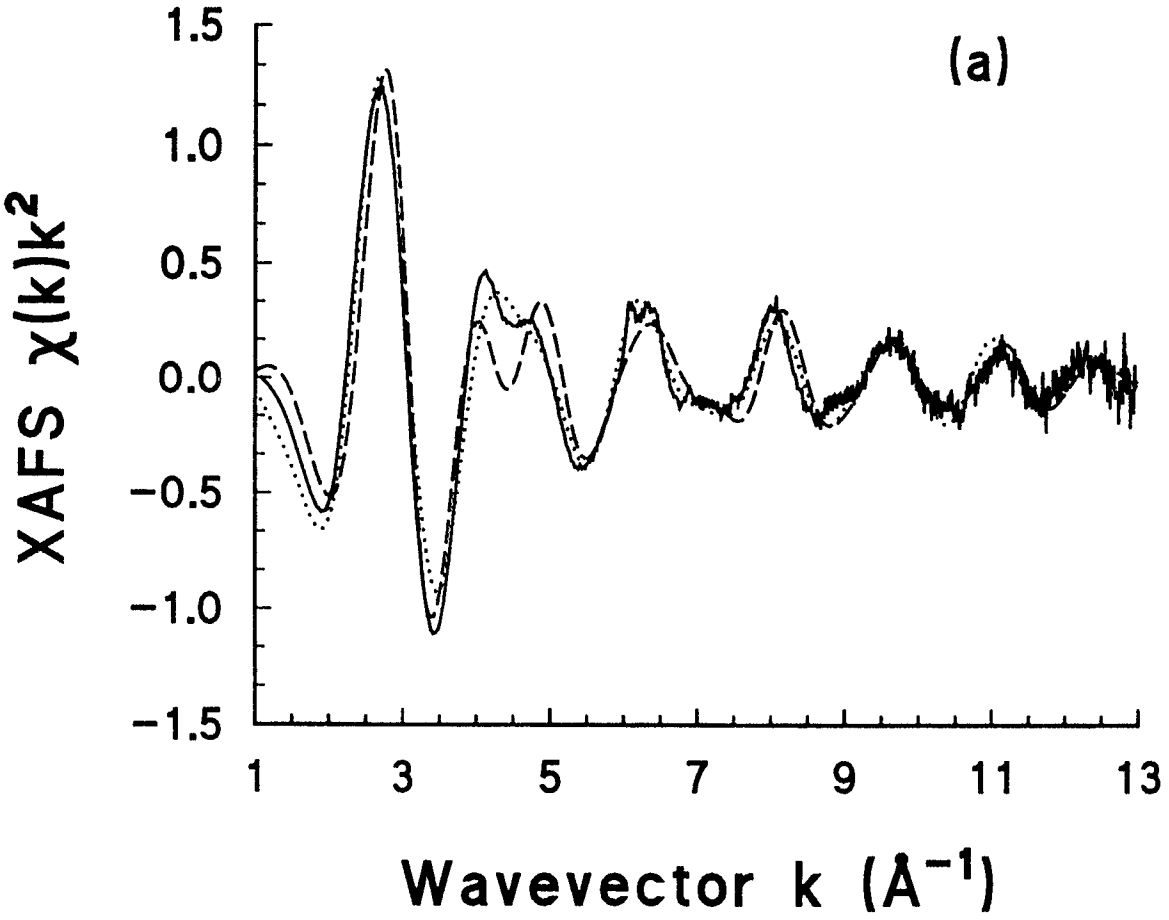

Figure S2a

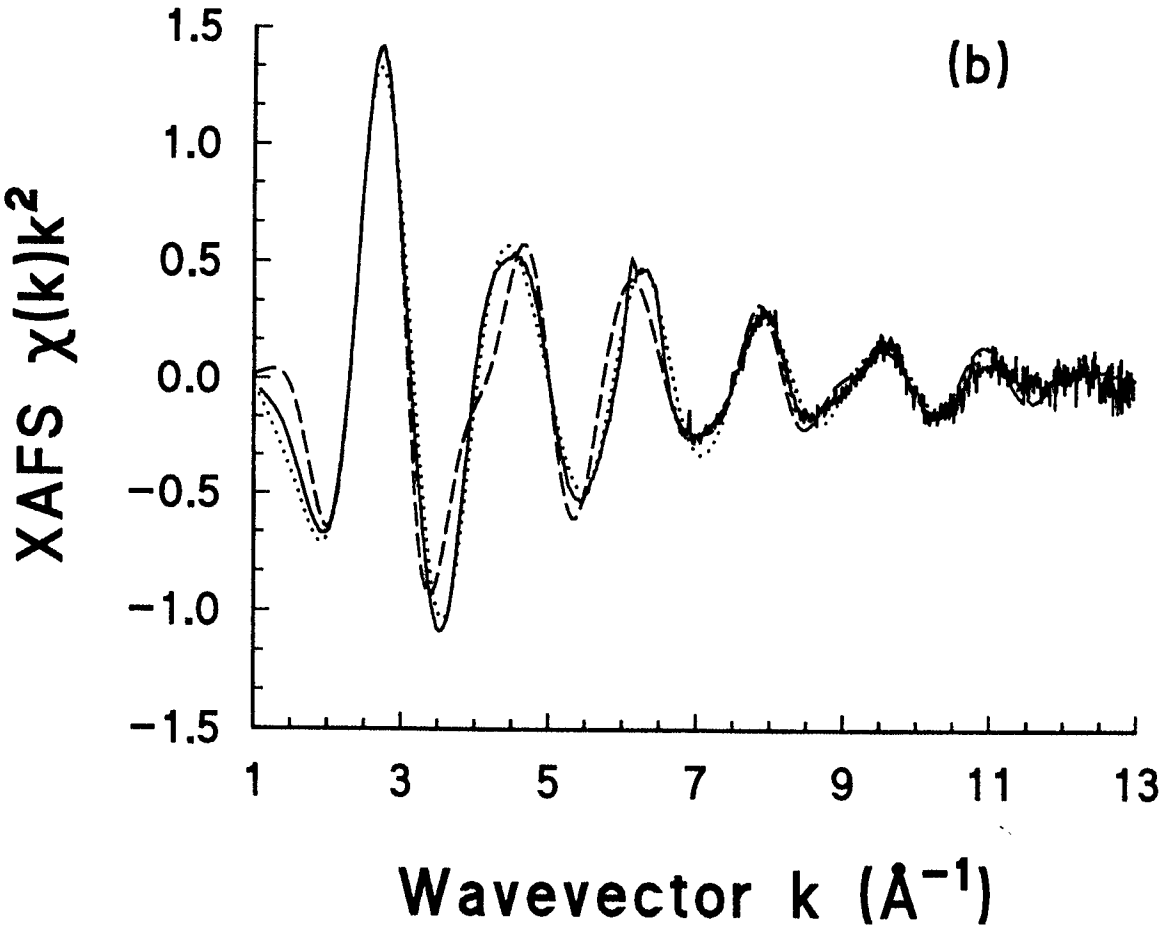

Figure S2b

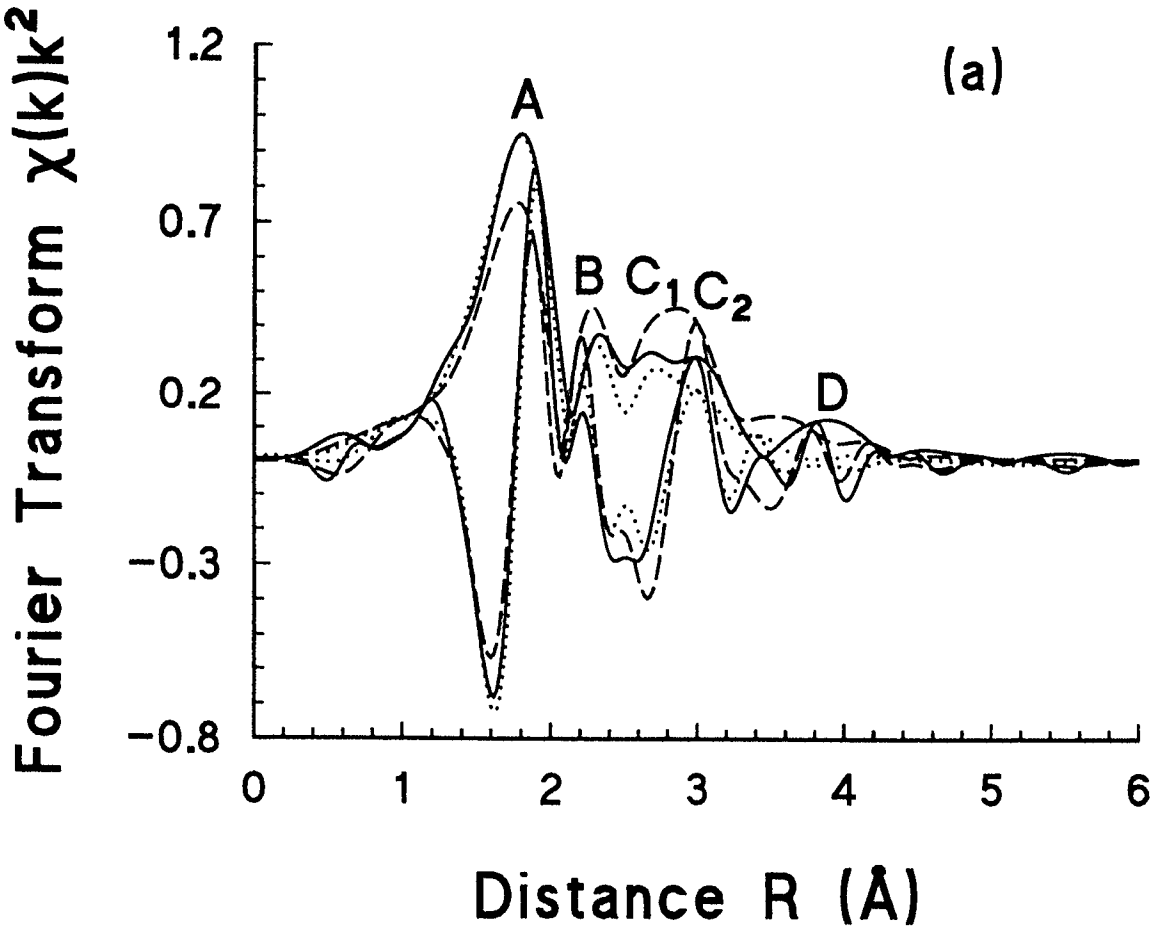
Fourier Transform χ(k)k²
1.2
0.7
0.2
−0.3
−0.8
0
1
2
3
4
5
6
Distance R (Å)
(a)
A
B
C1
C2
D

Figure S3a

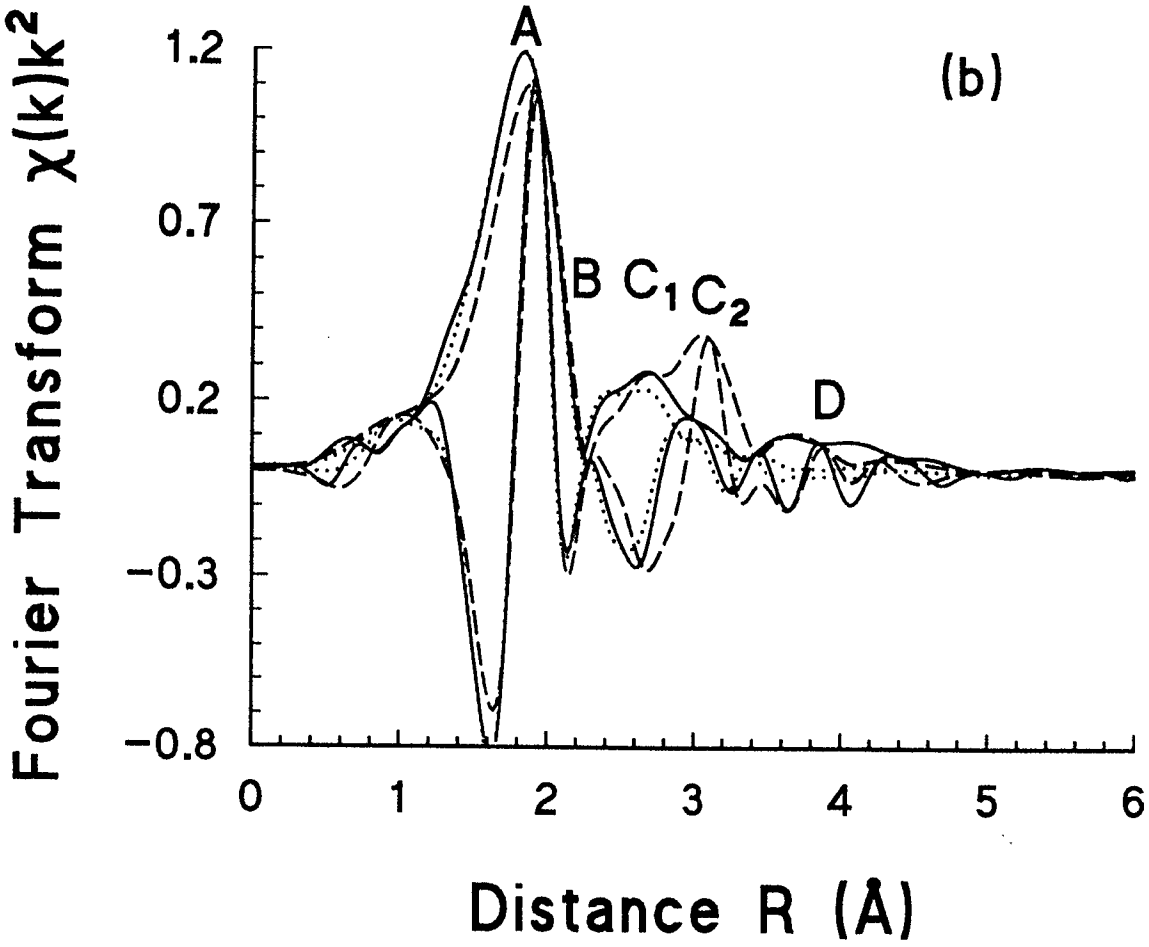
Fourier Transform χ(k)k²
1.2
0.7
0.2
−0.3
−0.8
0
1
2
3
4
5
6
A
B
C1
C2
D
(b)
Distance R (Å)

Figure S3b