Supporting Information

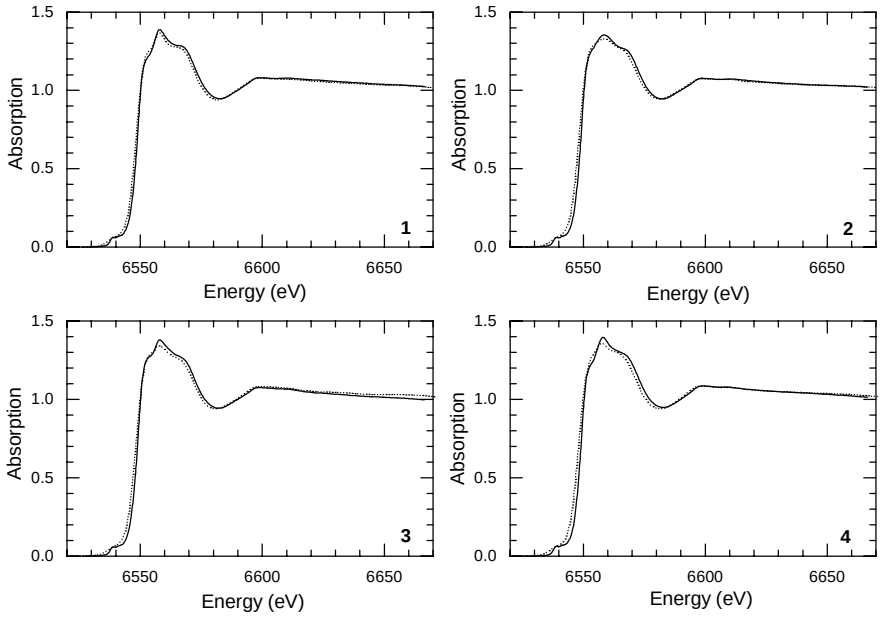

Figure S1. Comparison of the experimental XANES spectra (at room temperature) with the corresponding part of the experimental EXAFS spectra (at 10 K) (dotted line).

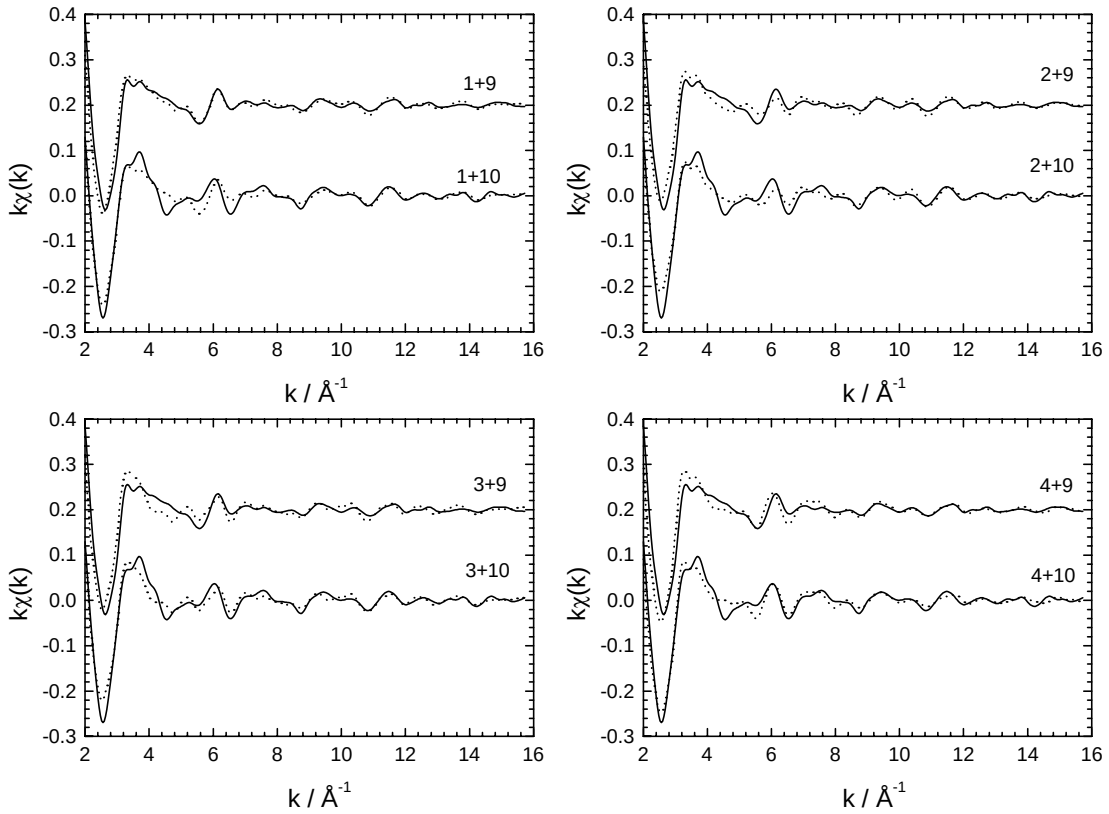

Figure S2. Comparison of the experimental EXAFS spectra of compounds **1** - **4** with the two model compounds **9** (with two coordinated water molecules) and **10** (with one hydroxo and one nitrate ions coordinated to the manganese centers).

Output files of EXAFS fitting

```
opened file:1-4c
number of shells : 4
scale (So)**2  : 1.00000
Variable mean free path lambda=[k+(eta/k)**4]/gamma

saved file :1-4c
eta value : 3.10000
valeur de Nind : 17
ech=  1.00000 ±  .000000
mean free patth = 1/gamma[k+(eta/k)**4]
eta=  3.10000 ±  .000000

N1   :  1.00000 ±  .000000
SIG1 :  5.820000E-02 ±  5.895703E-02
GAM1 :  .600000 ±  .000000
R1   :  1.78630 ±  5.000710E-03
DE1  :  -5.98000 ±  23.7973
N2   :  1.00000 ±  .000000
SIG2 :  6.700000E-02 ±  8.417670E-02
GAM2 :  .600000 ±  .000000
R2   :  1.95390 ±  5.770445E-03
DE2  :  -5.98000 ±  .000000
N3   :  2.00000 ±  .000000
SIG3 :  7.730000E-02 ±  6.909966E-02
GAM3 :  .600000 ±  .000000
R3   :  2.05800 ±  7.204413E-03
DE3  :  -5.98000 ±  .000000
N4   :  2.00000 ±  .000000
SIG4 :  .120400 ±  .124252
GAM4 :  .600000 ±  .000000
R4   :  2.22310 ±  5.564332E-03
DE4  :  -5.98000 ±  .000000

Residual =  2.606692E-02
weight = 1/sigma**2  , with sigma = A/k**n
A : 1.00000
n : .000000
Number of independent points : 17
Number of fitted parameters : 9
Degree of freedom : 8
Confidence interval : 1.00000
chi**2 : 4.345574E-04
Quality factor : 1.086394E-04
Correlation matrix :
C12
C13 C23
C14  C24  C34
 -1.948284E-02
 -1.971430E-02 -.108173
 2.426423E-02 .127814 .131969
 2.386695E-03 1.623530E-03 1.405345E-02 -1.486230E-02
 6.371226E-03 5.047136E-02 3.299545E-02 -4.415643E-02 -1.163404E-02
```

2.819980E-02 .152219 .153014 -.188528 -1.895254E-02 -4.887216E-02
-2.798298E-02 -.163314 -.150636 .188270 2.441479E-02 4.032864E-02 .216828
-8.218838E-03 -5.632676E-02 -4.342414E-02 5.610849E-02 1.099312E-02 6.277869E-03 6.337233E-02 -5.675240E-02

opened file:2-4c
number of shells : 4
scale (So)**2 : 1.00000
Variable mean free path lambda=[k+(eta/k)**4]/gamma

saved file :2-4c
eta value : 3.10000
valeur de Nind : 16
ech= 1.00000 ± .000000
mean free patth = 1/gamma[k+(eta/k)**4]
eta= 3.10000 ± .000000

N1 : 1.00000 ± .000000
SIG1 : 5.940000E-02 ± 6.070675E-02
GAM1 : .600000 ± .000000
R1 : 1.79210 ± 5.364537E-03
DE1 : -5.70000 ± 29.6538
N2 : 1.00000 ± .000000
SIG2 : 7.470000E-02 ± .110949
GAM2 : .600000 ± .000000
R2 : 1.96310 ± 7.806420E-03
DE2 : -5.70000 ± .000000
N3 : 2.00000 ± .000000
SIG3 : 8.010000E-02 ± 6.829196E-02
GAM3 : .600000 ± .000000
R3 : 2.06110 ± 5.951285E-03
DE3 : -5.70000 ± .000000
N4 : 2.00000 ± .000000
SIG4 : 9.470000E-02 ± .131399
GAM4 : .600000 ± .000000
R4 : 2.21850 ± 1.337397E-02
DE4 : -5.70000 ± .000000

Residual = 2.560154E-02
weight = 1/sigma**2 , with sigma = A/k**n
A : 1.00000
n : .000000
Number of independent points : 16
Number of fitted parameters : 9
Degree of freedom : 7
Confidence interval : 1.00000
chi**2 : 4.069082E-04
Quality factor : 8.138164E-05
Correlation matrix :
C12
C13 C23
C14 C24 C34
-8.852167E-02
-3.027978E-02 -8.153297E-02
5.718203E-02 .151552 4.734521E-02
-4.484870E-03 -1.382954E-02 -7.332895E-03 4.102888E-02

4.695412E-02 .126864 4.338429E-02 -8.181530E-02 6.508449E-03
4.150677E-02 .108902 3.230815E-02 -9.384852E-03 4.219423E-02 -5.933528E-02
-8.030040E-02 -.213680 -6.808197E-02 7.624781E-02 -4.799598E-02 .114933 3.145252E-02
-7.786980E-03 -1.930518E-02 -3.964494E-03 -2.007755E-02 -2.056006E-02 1.107871E-02 -2.716132E-02
1.843849E-02

opened file:3-4c
number of shells : 4
scale (So)**2 : 1.00000
Variable mean free path lambda=[k+(eta/k)**4]/gamma

saved file :3-4c
eta value : 3.10000
valeur de Nind : 16
ech= 1.00000 ± .000000
mean free patth = 1/gamma[k+(eta/k)**4]
eta= 3.10000 ± .000000

N1 : 1.00000 ± .000000
SIG1 : 6.160000E-02 ± 5.605152E-02
GAM1 : .600000 ± .000000
R1 : 1.79390 ± 7.761896E-03
DE1 : -5.77000 ± 23.6128
N2 : 1.00000 ± .000000
SIG2 : 6.190000E-02 ± 8.083805E-02
GAM2 : .600000 ± .000000
R2 : 1.96390 ± 4.525125E-03
DE2 : -5.77000 ± .000000
N3 : 2.00000 ± .000000
SIG3 : 7.040000E-02 ± 6.195193E-02
GAM3 : .600000 ± .000000
R3 : 2.07160 ± 7.781506E-03
DE3 : -5.77000 ± .000000
N4 : 2.00000 ± .000000
SIG4 : 9.050000E-02 ± .142799
GAM4 : .600000 ± .000000
R4 : 2.21610 ± 4.620910E-03
DE4 : -5.77000 ± .000000

Residual = 2.185947E-02
weight = 1/sigma**2 , with sigma = A/k**n
A : 1.00000
n : .000000
Number of independent points : 16
Number of fitted parameters : 10
Degree of freedom : 6
Confidence interval : 1.00000
chi**2 : 3.464120E-04
Quality factor : 5.773534E-05
Correlation matrix :
C12
C13 C23
C14 C24 C34
-3.943182E-02
-1.915678E-02 .123520
.186225 .129369 .120245

2.343210E-03 9.013738E-02 3.157219E-02 -4.667711E-02
.121795 -1.419912E-02 1.535062E-02 -.143531 .120610
9.702937E-02 7.964833E-02 .140477 -8.406778E-02 5.541397E-02 -.124361
-.168146 -.162001 -.261301 .149967 -6.288233E-02 .191127 1.779751E-02
-1.067919E-03 -.111640 -.174750 -4.905170E-02 2.494929E-02 -2.941345E-02 -9.934001E-02 .175427
1.576882E-03 -1.622539E-03 -8.741116E-03 1.250320E-02 2.158595E-02 -1.664324E-03 7.149987E-03 -1.251689E-02 -7.124298E-03
opened file:4-4c
number of shells : 4
scale (So)**2 : 1.00000
Variable mean free path lambda=[k+(eta/k)**4]/gamma

saved file :4-4c
eta value : 3.10000
valeur de Nind : 17
ech= 1.00000 ± .000000
mean free patth = 1/gamma[k+(eta/k)**4]
eta= 3.10000 ± .000000

N1 : 1.00000 ± .000000
SIG1 : 5.850000E-02 ± 7.689096E-02
GAM1 : .600000 ± .000000
R1 : 1.79390 ± 8.813024E-03
DE1 : -5.12000 ± 27.2577
N2 : 1.00000 ± .000000
SIG2 : 7.380000E-02 ± 7.923295E-02
GAM2 : .600000 ± .000000
R2 : 1.96190 ± 6.232679E-03
DE2 : -5.12000 ± .000000
N3 : 2.00000 ± .000000
SIG3 : 7.290000E-02 ± 8.893137E-02
GAM3 : .600000 ± .000000
R3 : 2.06660 ± 1.300108E-02
DE3 : -5.12000 ± .000000
N4 : 2.00000 ± .000000
SIG4 : .101500 ± .142329
GAM4 : .600000 ± .000000
R4 : 2.21750 ± 7.685065E-03
DE4 : -5.12000 ± .000000

Residual = 1.422707E-02
weight = 1/sigma**2 , with sigma = A/k**n
A : 1.00000
n : .000000
Number of independent points : 17
Number of fitted parameters : 9
Degree of freedom : 8
Confidence interval : 1.00000
chi**2 : 2.809440E-04
Quality factor : 4.013485E-05
Correlation matrix :
C12
C13 C23
C14 C24 C34
-.107368
-5.043530E-02 -9.762137E-02

5.412341E-03 .212142 .166541
-1.532090E-02 5.145944E-02 2.243538E-02 4.164016E-03
5.700280E-02 -1.617955E-02 5.776434E-02 -.109550 -1.830132E-02
6.730088E-03 .203751 .165302 -.114768 1.194425E-03 -.103076
-4.691125E-02 -.133727 -.166277 .169362 1.630107E-02 7.943999E-02 .167921
.101131 -3.958967E-02 6.198992E-03 -8.538790E-02 2.626516E-02 -8.771232E-02 -5.668185E-02
6.173422E-02