

## Supporting information

### Atomic-scale structure of gadolinium in nanocrystalline fluorapatite from marine sediments

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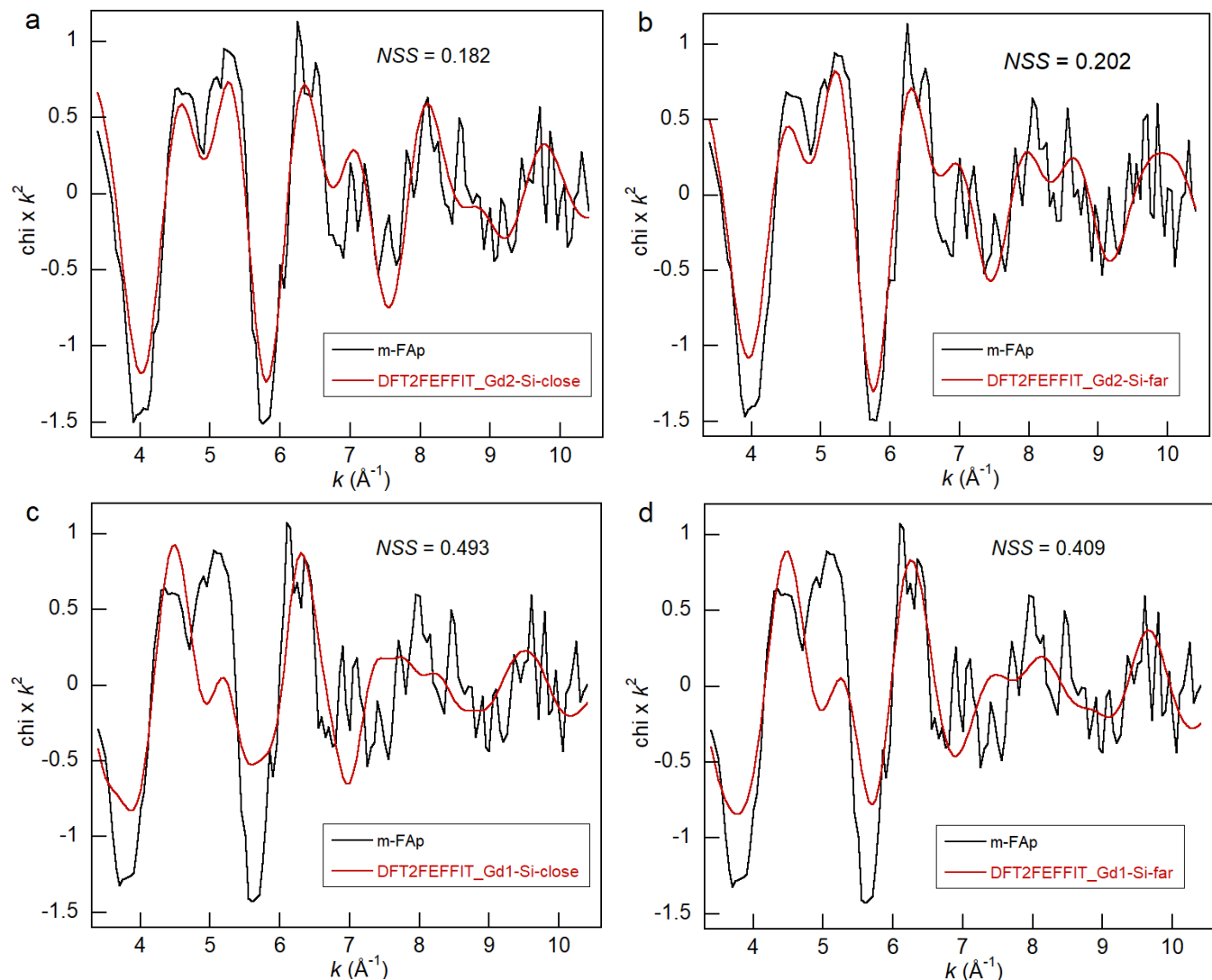
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#### 1. Supplementary tables

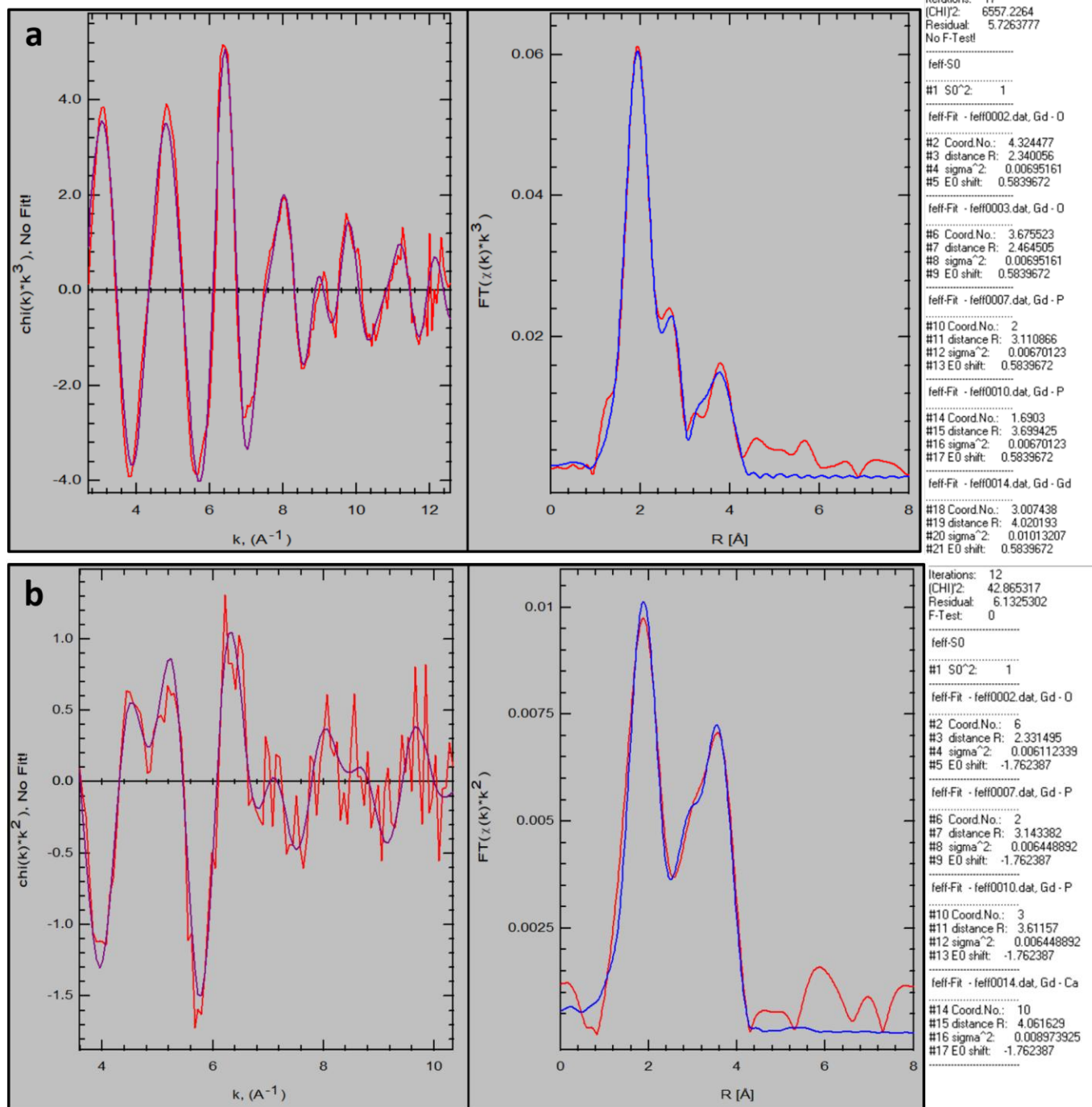
**Table S1.** Reaction affinities for the Gd(III) soluble species at 25°C used in Figure S7.

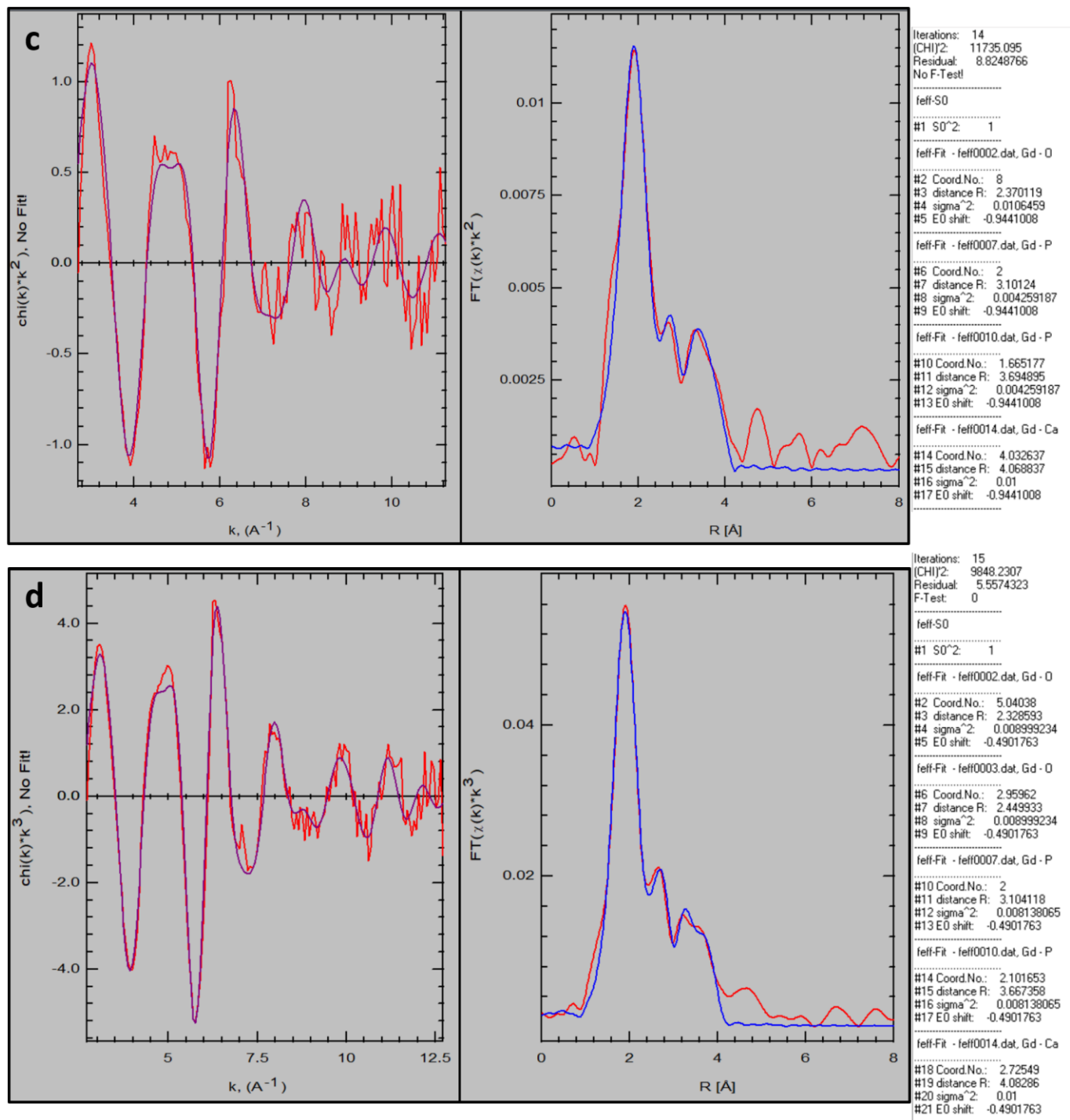
| Reaction                                                                                                    | logK   |
|-------------------------------------------------------------------------------------------------------------|--------|
| $\text{Gd}^{3+} + \text{H}_2\text{O} \leftrightarrow \text{GdOH}^{2+} + \text{H}^+$                         | -8.28  |
| $\text{Gd}^{3+} + \text{H}_2\text{O} \leftrightarrow \text{GdO}^+ + 2\text{H}^+$                            | -16.71 |
| $\text{Gd}^{3+} + 2\text{H}_2\text{O} \leftrightarrow \text{GdO}_2^+ + 4\text{H}^+$                         | -34.80 |
| $\text{Gd}^{3+} + 3\text{H}_2\text{O} \leftrightarrow \text{Gd}(\text{OH})_{3(\text{aq})} + 3\text{H}^+$    | -25.63 |
| $\text{Gd}^{3+} + \text{HCO}_3^- \leftrightarrow \text{GdCO}_3^+ + \text{H}^+$                              | -2.84  |
| $\text{Gd}^{3+} + 2\text{HCO}_3^- \leftrightarrow \text{Gd}(\text{CO}_3)_2^- + 2\text{H}^+$                 | -7.56  |
| $\text{Gd}^{3+} + \text{HCO}_3^- \leftrightarrow \text{GdHCO}_3^{+2}$                                       | 1.34   |
| $\text{Gd}^{3+} + \text{Cl}^- \leftrightarrow \text{GdCl}^{2+}$                                             | 0.31   |
| $\text{Gd}^{3+} + 2\text{Cl}^- \leftrightarrow \text{GdCl}_2^+$                                             | -0.04  |
| $\text{Gd}^{3+} + 3\text{Cl}^- \leftrightarrow \text{GdCl}_3$                                               | -0.47  |
| $\text{Gd}^{3+} + 4\text{Cl}^- \leftrightarrow \text{GdCl}_4^-$                                             | -0.89  |
| $\text{Gd}(\text{OH})_{3(\text{s})} + 3\text{H}^+ \leftrightarrow \text{Gd}^{3+} + 3\text{H}_2\text{O}$     | 15.59  |
| $\text{Gd}_2(\text{CO}_3)_{3(\text{s})} + 3\text{H}^+ \leftrightarrow 2\text{Gd}^{3+} + 3\text{HCO}_3^{2-}$ | -3.71  |

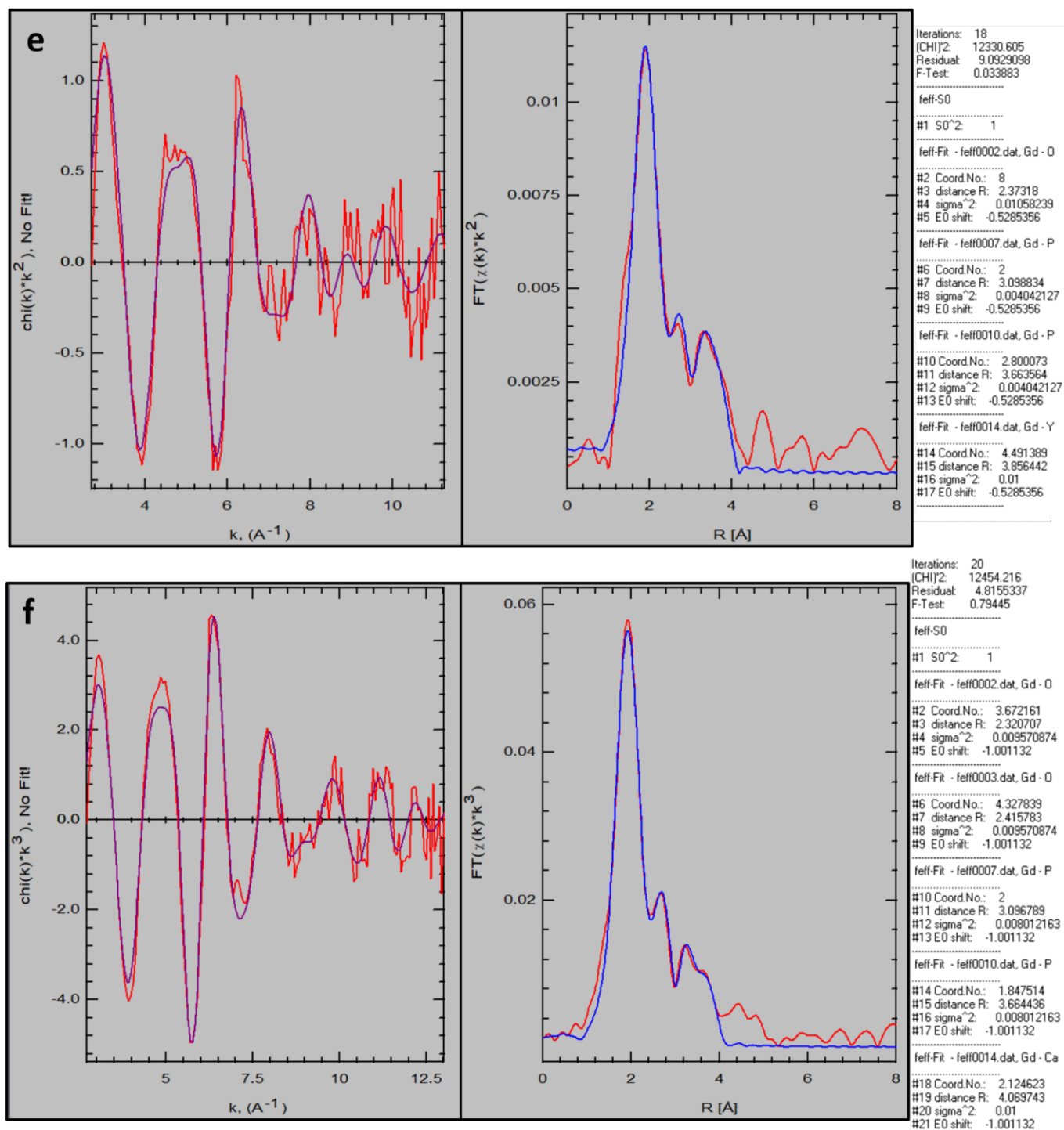
## 2. Supplementary figures



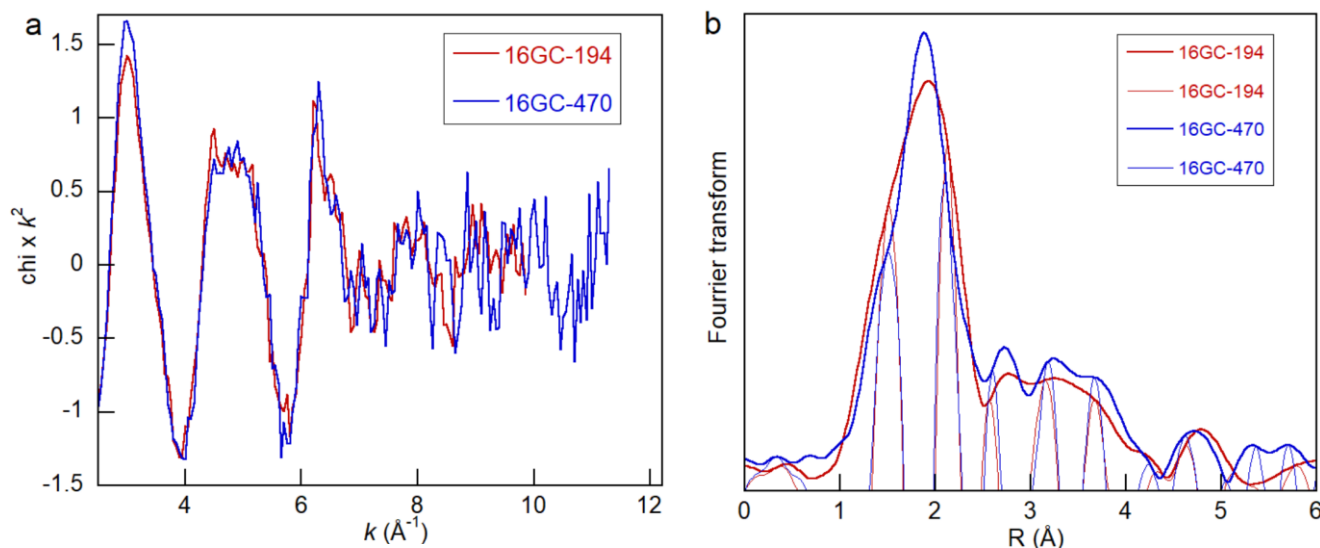
**Figure S1.** Experimental and p-DFT-derived theoretical Gd L<sub>3</sub>-edge EXAFS spectra obtained by DFT2FEFFIT<sup>1</sup> for hydrothermal FAp from Imilchil, Morocco (m-FAp). (a) Gd substituted in the Ca(2) site and charge excess balanced by a local Si for P substitution. (b) Gd substituted in the Ca(2) site and charge excess balanced by a distant Si for P substitution. (c) Gd substituted in the Ca(1) site and charge excess balanced by a local Si for P substitution. (d) Gd substituted in the Ca(1) site and charge excess balanced by a distant Si for P substitution. NSS is the fit residual expressed as the normalized sum of squared differences ( $NSS = \sum (k^3 \chi_{exp} - k^3 \chi_{calc})^2 / \sum (k^3 \chi_{exp})^2$ ). The input scripts and best-fit parameters of the DFT2FEFFIT calculations are given in section 4, the Cartesian coordinates of the four DFT models, taken from Dahbi et al. (2025),<sup>2</sup> are listed in section 5, and the EXAFS spectrum for m-FAp is given in section 6.



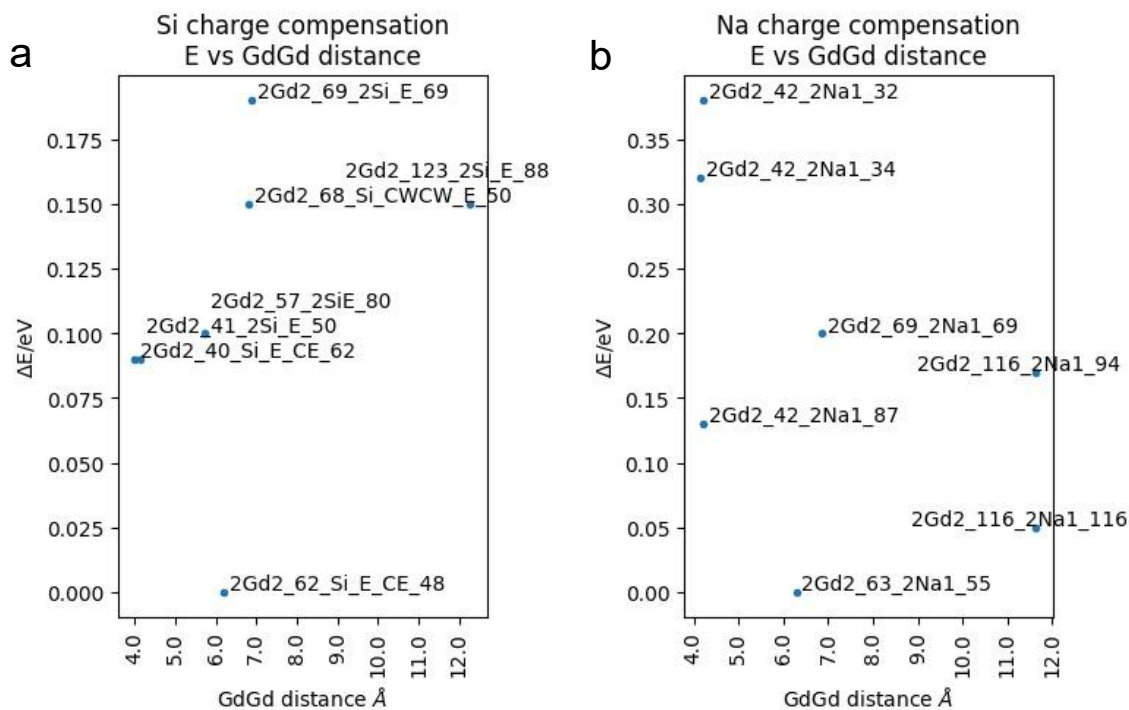




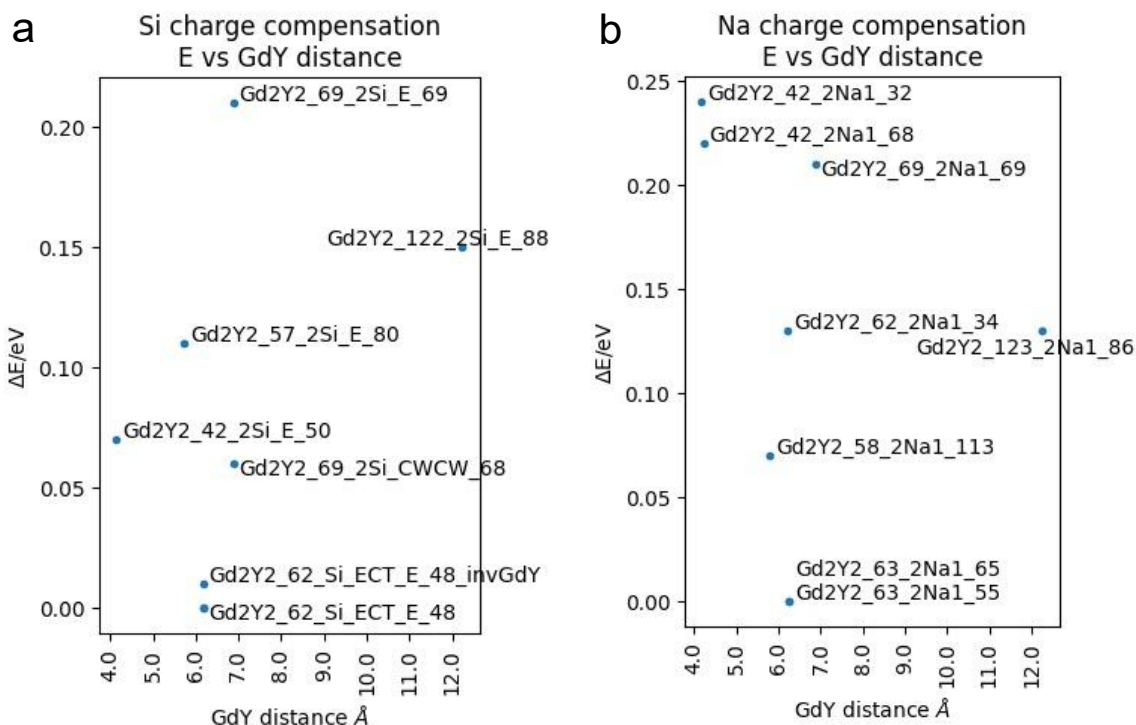
**Figure S2.** Best-fits of the EXAFS spectra. a) GdPO<sub>4</sub>·H<sub>2</sub>O.  $\Delta k = 10 \text{ Å}^{-1}$ ,  $\Delta R = 3.3 \text{ Å}$ , 12 free parameters. b) m-FAp.  $\Delta k = 6.7 \text{ Å}^{-1}$ ,  $\Delta R = 3.2 \text{ Å}$ , 8 free parameters. c) b-CFA, Gd-Ca model.  $\Delta k = 8.4 \text{ Å}^{-1}$ ,  $\Delta R = 3.2 \text{ Å}$ , 9 free parameters. d) Gd-HAp.  $\Delta k = 10.0 \text{ Å}^{-1}$ ,  $\Delta R = 3.3 \text{ Å}$ , 11 free parameters. e) b-CFA, Gd-Y model.  $\Delta k = 10.0 \text{ Å}^{-1}$ ,  $\Delta R = 3.3 \text{ Å}$ , 11 free parameters. f) Gd,Y-HAp.  $\Delta k = 10.1 \text{ Å}^{-1}$ ,  $\Delta R = 3.1 \text{ Å}$ , 11 free parameters.



**Figure S3.** Gd L3-edge EXAFS spectra (a) and Fourier transforms (modulus and imaginary parts) (b) of the two b-CFA samples collected at 1.94 m (16GC-194, [Gd] = 1548 mg/kg) and 4.70 m (16GC-470, [Gd] = 1756 mg/kg) below the seafloor.



**Figure S4.** Relative energies of Gd(2)-Gd(2) Fap structures as a function of the Gd-Gd distance. Supercell size:  $2 \times 2 \times 2$ . (a) Charge balance: Si for P substitution. (b) Charge balance: Na(1) for Ca(1) substitution. The tag structure for the filenames is explained below.



**Figure S5.** Relative energies of Gd(2)-Y(2) FAp structures as a function of the Gd-Y distance. Supercell size:  $2 \times 2 \times 2$ . (a) Charge balance: Si for P substitution. (b) Charge balance: Na(1) for Ca(1) substitution

#### Tag structure of the REY\_dist<sub>REY-REY</sub>\_Cc(\_CcID)\_dist<sub>Cc-Cc</sub> filenames in Figures S4 and S5.

“REY” stands for the REY element in the FAp structure, followed by the site it occupies. 2Gd2 means that the supercell contains two Gd atoms in the Ca(2) site. Gd2Y2 means that the supercell contains one Gd and one Y atom, both in a Ca(2) site.

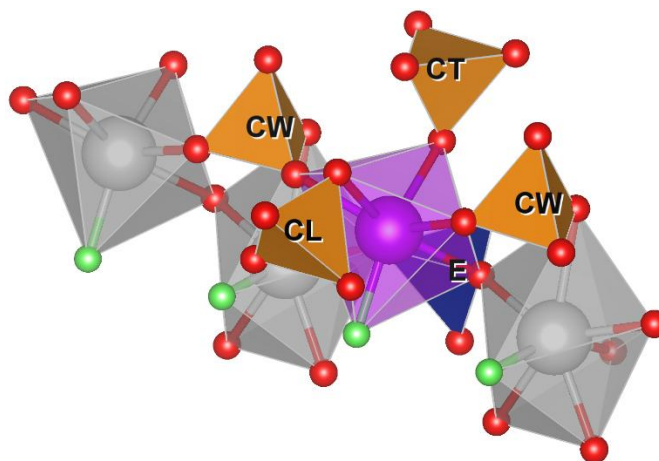
“dist<sub>REY-REY</sub>” is the distance separation between the two REY atoms, considering periodic boundary conditions in tenth of Å.

“Cc” is the charge compensation mechanism, which is Si in the case of  $\text{Si}^{4+}$  for  $\text{P}^{5+}$  substitution and Na1 in the case of  $\text{Na}^+$  for  $\text{Ca}^{2+}$ (1) substitution.

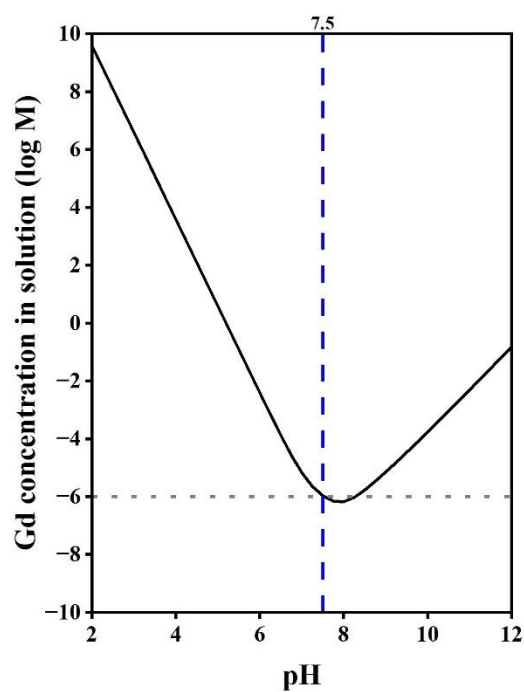
“CcID” is present when Cc=Si to specify the position and linkage type of each silicate tetrahedron. The tag starts with a C for a corner connection and with an E for an edge connection to the  $\text{REYO}_6\text{F}$  polyhedron. Since the C and E tags are insufficient to differentiate all possible arrangements, an additional letter is added in case of a corner connection (Figure S6). W symbolizes a tetrahedron connected to two Ca(2) sites along the FAp channel. T represents the tetrahedron away from the FAp channel. L represents the tetrahedron closer to the FAp channel. When each tetrahedron has the same bonding environment, a unique “CcID” is present (e.g., Gd2Y2\_69\_2Si\_CWCW\_68). Otherwise, the two distinct bonding environments are separated by an underscore. One can notice the absence of the “2” before Si in such cases (e.g., Gd2Y2\_62\_Si\_ECT\_E\_48).

“dist<sub>Cc-Cc</sub>” specifies the distance between the two Na or Si atoms in tenths of Å.

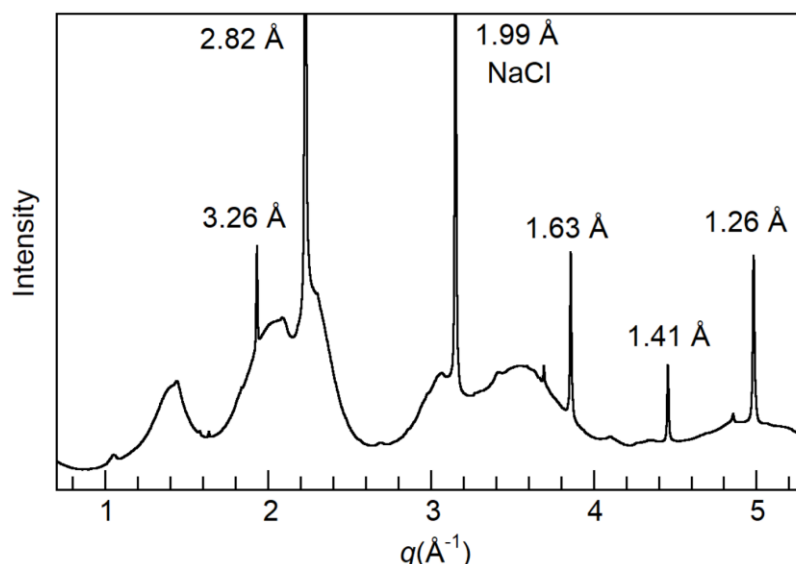
The invGdY tag indicates that the Gd and Y positions were exchanged with respect to the same structure without tag. The Gd2Y2\_62\_Si\_ECT\_48 and Gd2Y2\_62\_Si\_ECT\_48\_invGdY configurations are almost isoenergetic, and therefore, Gd-Y inversion was not repeated for other structures.



**Figure S6.** Coordination of a  $\text{GdO}_6\text{F}$  polyhedron in the Ca(2) site of FAp with a Si for P substitution at short distance. Gd, purple, Ca, gray; O, red; F, green;  $\text{PO}_4^{3-}$  tetrahedron, light brown;  $\text{SiO}_4^{4-}$  tetrahedron, blue.



**Figure S7.** Gd(III) solubility diagram (M, logarithmic scale) at atmospheric  $p\text{CO}_2$  (with carbonates in solution), using data from the Lawrence Livermore National Laboratory database (Table S1). The blue dashed line denotes the experimental pH 7.5. Gd concentrations in solution were at the  $\mu\text{M}$  level (gray line).



**Figure S8.** XRD pattern of  $\text{GdPO}_4 \cdot \text{H}_2\text{O}$  measured on beamline ID22 at the European Synchrotron Radiation Facility (ESRF). The sharp lines are from NaCl. Na comes from NaOH and Cl from  $\text{GdCl}_3$ . The phase was identified after the XRD pattern of Lessing et al. (2003).<sup>3</sup>

### S3. References

- 1 A. Manceau, R. Brossier, O. Mathon, K. A. Lomachenko, M. Retegan, P. Glatzel and S. N. Steinmann, DFT2FEFFIT: a density-functional-theory-based structural toolkit to analyze EXAFS spectra, *J. Appl. Cryst.*, 2024, **57**, 1229–1234.
- 2 S. Dahbi, A. Rosa, A. Manceau and S. N. Steinmann, Prediction and Rationalization of Site Preference of Rare Earth Elements in Fluorapatite from Density Functional Theory, *ACS Earth Space Chem.*, 2025, **9**, 1633–1641.
- 3 P. A. Lessing and A. W. Erickson, Synthesis and characterization of gadolinium phosphate neutron absorber, *J. Eur. Ceram. Soc.*, 2003, **23**, 3049–3057.

### S4. Input scripts and best-fit parameters of the DFT2FEFFIT calculations

#### S4.1. Gd2-Si-close

```
m-FAp.chi
19
2
3.4 10.4
0.9
1
-0.5 1.8 0.3
1; F;2.27;chip0001.dat;FEFF;1;0.06; 0.02; 0.13; -1
2; 2O;2.32;chip0002.dat;FEFF;1; 0.06;0.02; 0.13; 1
3; 2O;2.33;chip0003.dat;FEFF;1; 0.06;0.02; 0.13; 1
4; O;2.34;chip0004.dat;FEFF;1; 0.06;0.02; 0.13; 1
5; O;2.69;chip0005.dat;FEFF;1; 0.06;0.02; 0.13; 1
6; Si;2.99;chip0006.dat;FEFF;1; 0.06;0.02; 0.13;-1
7; P;3.29;chip0007.dat;FEFF;1; 0.06; 0.02; 0.13; 6
10; P;3.53;chip0010.dat;FEFF;1;0.06; 0.02; 0.13; -1
12; 2P;3.69;chip0012.dat;FEFF;1;0.06; 0.02; 0.13; 10
14; Ca;3.96;chip0014.dat;FEFF;1;0.06; 0.02; 0.13; -1
17; Ca;4.00;chip0017.dat;FEFF;1;0.06; 0.02; 0.13; 14
```

18; Ca;4.00;chip0018.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 19; Ca;4.04;chip0019.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 20; Ca;4.05;chip0020.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 21; Ca;4.05;chip0021.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 22; 2Ca;4.10;chip0022.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 25; Ca;4.18;chip0025.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 26; Ca;4.18;chip0026.dat;FEFF;1;0.06; 0.02; 0.13; 14  
 27; MS;2.31;Gd2-Si-close\_MS.chi;2C;1;0.13; 0.08; 0.17; -1

Best-fit parameters:

$\Delta E = 1.6$  eV;  $\sigma(\text{O,F}) = 0.07$  Å;  $\sigma(\text{Si,P1}) = 0.13$  Å;  $\sigma(\text{P2}) = 0.02$  Å;  $\sigma(\text{Ca}) = 0.06$  Å; ;  $\sigma(\text{MS}) = 0.17$  Å;  $NSS = 0.182$

## S4.2. Gd2-Si-far

m-FAp

22

2

3.4 10.4

0.9

1

0.5 2.0 0.3

1; F;2.25;chip0001.dat;FEFF;1;0.06; 0.02; 0.13; -1  
 2; 2O;2.29;chip0002.dat;FEFF;1; 0.06;0.02; 0.13; 1  
 3; O;2.33;chip0003.dat;FEFF;1; 0.06;0.02; 0.13; 1  
 4; O;2.42;chip0004.dat;FEFF;1; 0.06;0.02; 0.13; 1  
 5; O;2.42;chip0005.dat;FEFF;1; 0.06;0.02; 0.13; 1  
 6; O;2.58;chip0006.dat;FEFF;1; 0.06;0.02; 0.13; 1  
 7; P;3.05;chip0007.dat;FEFF;1; 0.06; 0.02; 0.13; -1  
 8; P;3.18;chip0008.dat;FEFF;1;0.06; 0.02; 0.13; 7  
 12; P;3.49;chip0012.dat;FEFF;1;0.06; 0.02; 0.13; -1  
 13; P;3.67;chip0013.dat;FEFF;1;0.06; 0.02; 0.13; 12  
 14; P;3.67;chip0014.dat;FEFF;1;0.06; 0.02; 0.13; 12  
 17; Ca;4.00;chip0017.dat;FEFF;1;0.06; 0.02; 0.13; -1  
 18; Ca;4.01;chip0018.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 19; Ca;4.01;chip0019.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 20; Ca;4.07;chip0020.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 23; Ca;4.10;chip0023.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 24; Ca;4.11;chip0024.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 25; Ca;4.15;chip0025.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 26; Ca;4.15;chip0026.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 27; Ca;4.19;chip0027.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 28; Ca;4.19;chip0028.dat;FEFF;1;0.06; 0.02; 0.13; 17  
 29; MS;2.31;Gd2-Si-far\_MS.chi;2C;1;0.13; 0.08; 0.17; -1

Best-fit parameters:

$\Delta E = 0.8$  eV;  $\sigma(\text{O,F}) = 0.03$  Å;  $\sigma(\text{Si,P1}) = 0.04$  Å;  $\sigma(\text{P2}) = 0.02$  Å;  $\sigma(\text{Ca}) = 0.06$  Å; ;  $\sigma(\text{MS}) = 0.17$  Å;  $NSS = 0.203$

## S4.3. Gd1-Si-close

m-FAp

24

2

3.4 10.4

0.9

1

-6.5 -2.0 0.3

1; F;2.35;chip0001.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 2; O;2.37;chip0002.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 3; O;2.39;chip0003.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 4; O;2.43;chip0004.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 5; O;2.45;chip0005.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 6; O;2.48;chip0006.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 7; O;2.48;chip0007.dat;FEFF;1; 0.06; 0.04; 0.10; 1  
 8; O;2.64;chip0008.dat;FEFF;1; 0.06; 0.04; 0.10; 1  
 9; O;2.69;chip0009.dat;FEFF;1; 0.06; 0.04; 0.10; 1  
 10; Si;3.09;chip0010.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 11; P;3.18;chip0011.dat;FEFF;1;0.06; 0.04; 0.10; 10  
 12; P;3.20;chip0012.dat;FEFF;1;0.06; 0.04; 0.10; 10  
 13; Ca;3.44;chip0013.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 14; Ca;3.53;chip0014.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 15; P;3.57;chip0015.dat;FEFF;1;0.06; 0.04; 0.10; -1  
 16; P;3.60;chip0016.dat;FEFF;1;0.06; 0.04; 0.10; 15  
 17; P;3.67;chip0017.dat;FEFF;1;0.06; 0.04; 0.10; 15  
 20; Ca;3.92;chip0020.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 21; Ca;3.94;chip0021.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 24; Ca;3.99;chip0024.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 25; Ca;4.04;chip0025.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 27; Ca;4.08;chip0027.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 29; Ca;4.10;chip0029.dat;FEFF;1;0.06; 0.04; 0.10; 13  
 100; MS;2.31;chi\_MS.dat;2C;1;0.10; 0.07; 0.17; -1

Best-fit parameters:

$\Delta E = -5.0$  eV;  $\sigma(\text{O},\text{F}) = 0.07$  Å;  $\sigma(\text{Si},\text{P1}) = 0.07$  Å;  $\sigma(\text{P2}) = 0.10$  Å;  $\sigma(\text{Ca}) = 0.12$  Å; ;  $\sigma(\text{MS}) = 0.12$  Å;  $NSS = 0.493$

#### S4.4. Gd1-Si-far

m-Fap

23

2

3.4 10.4

0.9

1

-6.5 -2 0.3

1; F;2.35;chip0001.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 2; O;2.36;chip0002.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 3; O;2.36;chip0003.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 4; O;2.43;chip0004.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 5; O;2.43;chip0005.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 6; O;2.44;chip0006.dat;FEFF;1; 0.06;0.04; 0.10; 1  
 7; O;2.61;chip0007.dat;FEFF;1; 0.06; 0.04; 0.10; 1  
 8; O;2.61;chip0008.dat;FEFF;1; 0.06; 0.04; 0.10; 1  
 9; O;2.62;chip0009.dat;FEFF;1; 0.06; 0.04; 0.10; 1  
 10; 2P;3.16;chip0010.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 11; P;3.16;chip0011.dat;FEFF;1;0.06; 0.04; 0.10; 10  
 12; Ca;3.48;chip0012.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 13; Ca;3.50;chip0013.dat;FEFF;1;0.06; 0.04; 0.10; 12  
 14; P;3.58;chip0014.dat;FEFF;1;0.06; 0.04; 0.12; -1  
 15; P;3.59;chip0015.dat;FEFF;1;0.06; 0.04; 0.10; 14  
 16; P;3.59;chip0016.dat;FEFF;1;0.06; 0.04; 0.10; 14  
 21; Ca;4.02;chip0021.dat;FEFF;1;0.06; 0.04; 0.10; 12

22; Ca;4.02;chip0022.dat;FEFF;1;0.06; 0.04; 0.10; 12  
 24; Ca;4.03;chip0024.dat;FEFF;1;0.06; 0.04; 0.10; 12  
 25; Ca;4.06;chip0025.dat;FEFF;1;0.06; 0.04; 0.10; 12  
 26; Ca;4.06;chip0026.dat;FEFF;1;0.06; 0.04; 0.10; 12  
 27; Ca;4.06;chip0027.dat;FEFF;1;0.06; 0.04; 0.10; 12  
 100; MS;2.31;chi\_MS.dat;2C;1;0.10; 0.07; 0.17; -1

Best-fit parameters:

$\Delta E = -5.0$  eV;  $\sigma(\text{O,F}) = 0.05$  Å;  $\sigma(\text{Si,P1}) = 0.09$  Å;  $\sigma(\text{P2}) = 0.12$  Å;  $\sigma(\text{Ca}) = 0.11$  Å; ;  $\sigma(\text{MS}) = 0.08$  Å;  $NSS = 0.409$

## S5. Cartesian coordinates of the DFT2FEFFIT models

### S5.1. Gd2-Si-close

|    |              |              |              |
|----|--------------|--------------|--------------|
| 64 | 5.853630458  | 10.117814888 | 5.141569250  |
| 14 | 8.268044305  | 8.354036429  | 5.141144081  |
| 20 | 9.359860896  | 5.434314337  | 3.452140667  |
| 20 | 9.365173542  | 5.433899926  | 6.821610016  |
| 20 | 5.940265009  | 6.154073886  | 5.142533665  |
| 20 | 4.689555203  | 2.702275919  | 13.739939893 |
| 20 | 4.706098895  | 2.712782639  | 6.868598830  |
| 20 | 14.082753643 | 2.722095390  | 13.742371483 |
| 20 | 14.071937680 | 2.728122149  | 6.865216789  |
| 20 | 0.003495623  | 10.847810327 | 13.742111393 |
| 20 | -0.009149948 | 10.856014321 | 6.867777747  |
| 20 | 9.390208270  | 10.852532430 | 13.745713940 |
| 20 | 9.404176305  | 10.795013248 | 6.848405040  |
| 20 | 0.014294842  | 5.426540211  | 6.852493862  |
| 20 | -0.000831110 | 5.425488506  | 13.725812723 |
| 20 | 9.383683575  | 5.431512889  | 13.736347970 |
| 20 | -4.694655751 | 13.565772839 | 6.851409309  |
| 20 | -4.695899502 | 13.554241033 | 13.725745182 |
| 20 | 4.691294297  | 13.597496492 | 6.859144006  |
| 20 | 4.685950788  | 13.581066829 | 13.724879544 |
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## S6. EXAFS spectra

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| 10.400000 | -0.11084168E-02 |
| 10.450000 | -0.68169168E-03 |
| 10.500000 | -0.69272292E-03 |
| 10.550000 | -0.92358292E-03 |

|           |                 |
|-----------|-----------------|
| 10.600000 | -0.72008573E-03 |
| 10.650000 | -0.60419446E-03 |
| 10.700000 | -0.13466810E-03 |
| 10.750000 | -0.33282949E-03 |
| 10.800000 | 0.93678484E-04  |
| 10.850000 | -0.33113679E-03 |
| 10.900000 | 0.11986500E-03  |
| 10.950000 | 0.98304617E-04  |
| 11.000000 | 0.41549111E-03  |
| 11.050000 | 0.37979161E-03  |
| 11.100000 | 0.42228356E-03  |
| 11.150000 | 0.53193954E-03  |
| 11.200000 | 0.39272474E-03  |
| 11.250000 | 0.81223833E-03  |
| 11.300000 | 0.88806898E-03  |
| 11.350000 | 0.48819607E-03  |
| 11.400000 | 0.20756528E-03  |
| 11.450000 | 0.26178204E-03  |
| 11.500000 | -0.40155684E-03 |
| 11.550000 | -0.34155610E-03 |
| 11.600000 | -0.41855182E-03 |
| 11.650000 | -0.65847173E-03 |
| 11.700000 | -0.72782610E-03 |
| 11.750000 | -0.48215776E-03 |
| 11.800000 | -0.65312763E-03 |
| 11.850000 | -0.21954078E-03 |
| 11.900000 | -0.34823730E-03 |
| 11.950000 | -0.53869779E-03 |
| 12.000000 | 0.73692666E-03  |
| 12.050000 | -0.24721864E-03 |
| 12.100000 | -0.34786282E-03 |
| 12.150000 | 0.98685495E-04  |
| 12.200000 | -0.17146066E-03 |
| 12.250000 | 0.13035281E-03  |
| 12.300000 | 0.55623845E-03  |
| 12.350000 | 0.48059773E-03  |
| 12.400000 | 0.12474766E-03  |
| 12.450000 | 0.11237578E-03  |
| 12.500000 | 0.38555356E-04  |
| 12.550000 | 0.53269363E-04  |
| 12.600000 | 0.13657720E-03  |

## S6.2. m-FAp

|        |           |
|--------|-----------|
| 1.9000 | 0.10850   |
| 1.9500 | 0.10143   |
| 2.0000 | 0.070470  |
| 2.0500 | 0.027412  |
| 2.1000 | -0.012563 |
| 2.1500 | -0.063974 |
| 2.2000 | -0.097647 |
| 2.2500 | -0.12911  |
| 2.3000 | -0.13282  |
| 2.3500 | -0.13554  |

|        |             |
|--------|-------------|
| 2.4000 | -0.14286    |
| 2.4500 | -0.13287    |
| 2.5000 | -0.11567    |
| 2.5500 | -0.099759   |
| 2.6000 | -0.066621   |
| 2.6500 | -0.031426   |
| 2.7000 | -0.0031010  |
| 2.7500 | 0.049641    |
| 2.8000 | 0.10189     |
| 2.8500 | 0.12918     |
| 2.9000 | 0.15541     |
| 2.9500 | 0.16408     |
| 3.0000 | 0.15435     |
| 3.0500 | 0.12329     |
| 3.1000 | 0.10658     |
| 3.1500 | 0.089551    |
| 3.2000 | 0.061464    |
| 3.2500 | 0.042170    |
| 3.3000 | 0.038325    |
| 3.3500 | 0.035111    |
| 3.4000 | 0.021750    |
| 3.4500 | 0.012412    |
| 3.5000 | 0.013750    |
| 3.5500 | 0.023249    |
| 3.6000 | -0.00083210 |
| 3.6500 | -0.0060337  |
| 3.7000 | -0.014609   |
| 3.7500 | -0.040863   |
| 3.8000 | -0.057690   |
| 3.8500 | -0.078442   |
| 3.9000 | -0.072369   |
| 3.9500 | -0.071284   |
| 4.0000 | -0.069410   |
| 4.0500 | -0.069905   |
| 4.1000 | -0.062740   |
| 4.1500 | -0.041329   |
| 4.2000 | -0.038357   |
| 4.2500 | -0.021963   |
| 4.3000 | -0.0011908  |
| 4.3500 | 0.015569    |
| 4.4000 | 0.025820    |
| 4.4500 | 0.032921    |
| 4.5000 | 0.031327    |
| 4.5500 | 0.026845    |
| 4.6000 | 0.025417    |
| 4.6500 | 0.023366    |
| 4.7000 | 0.020790    |
| 4.7500 | 0.013473    |
| 4.8000 | 0.0047420   |
| 4.8500 | -0.00055593 |
| 4.9000 | 0.0099009   |
| 4.9500 | 0.015628    |
| 5.0000 | 0.017980    |

|        |            |
|--------|------------|
| 5.0500 | 0.019187   |
| 5.1000 | 0.012656   |
| 5.1500 | 0.024308   |
| 5.2000 | 0.023329   |
| 5.2500 | 0.022225   |
| 5.3000 | 0.022337   |
| 5.3500 | 0.016472   |
| 5.4000 | 0.017434   |
| 5.4500 | 0.0032841  |
| 5.5000 | -0.0090962 |
| 5.5500 | -0.036547  |
| 5.6000 | -0.031805  |
| 5.6500 | -0.050951  |
| 5.7000 | -0.051039  |
| 5.7500 | -0.048114  |
| 5.8000 | -0.048005  |
| 5.8500 | -0.039518  |
| 5.9000 | -0.033433  |
| 5.9500 | -0.011812  |
| 6.0000 | -0.018631  |
| 6.0500 | -0.013811  |
| 6.1000 | 0.0028122  |
| 6.1500 | 0.013381   |
| 6.2000 | 0.030432   |
| 6.2500 | 0.031153   |
| 6.3000 | 0.018094   |
| 6.3500 | 0.020428   |
| 6.4000 | 0.015188   |
| 6.4500 | 0.023849   |
| 6.5000 | 0.022525   |
| 6.5500 | 0.019402   |
| 6.6000 | 0.0074591  |
| 6.6500 | -0.0035696 |
| 6.7000 | -0.0017184 |
| 6.7500 | -0.0050688 |
| 6.8000 | -0.0033486 |
| 6.8500 | -0.0067070 |
| 6.9000 | -0.0060971 |
| 6.9500 | 0.0048851  |
| 7.0000 | 0.0074404  |
| 7.0500 | -0.0024607 |
| 7.1000 | -0.0053331 |
| 7.1500 | 0.0046766  |
| 7.2000 | 0.0040000  |
| 7.2500 | -0.0021917 |
| 7.3000 | -0.0040801 |
| 7.3500 | -0.012198  |
| 7.4000 | -0.0071891 |
| 7.4500 | -0.0080017 |
| 7.5000 | -0.0013451 |
| 7.5500 | -0.0065488 |
| 7.6000 | -0.0083936 |
| 7.6500 | -0.010743  |

|        |             |
|--------|-------------|
| 7.7000 | -0.0061038  |
| 7.7500 | 0.0022292   |
| 7.8000 | 0.0036816   |
| 7.8500 | -0.00094240 |
| 7.9000 | -0.0036209  |
| 7.9500 | 0.0031288   |
| 8.0000 | 0.0049899   |
| 8.0500 | 0.0093883   |
| 8.1000 | 0.0064943   |
| 8.1500 | 0.0020026   |
| 8.2000 | 0.0034709   |
| 8.2500 | 0.0039647   |
| 8.3000 | -0.0042510  |
| 8.3500 | 0.00038442  |
| 8.4000 | -0.0045248  |
| 8.4500 | -0.0025247  |
| 8.5000 | 0.0040940   |
| 8.5500 | 0.0086117   |
| 8.6000 | 0.0027833   |
| 8.6500 | -0.0012420  |
| 8.7000 | 0.0010946   |
| 8.7500 | -0.0023467  |
| 8.8000 | 0.0026739   |
| 8.8500 | -0.0022276  |
| 8.9000 | -0.0058202  |
| 8.9500 | 0.0014259   |
| 9.0000 | -0.0022407  |
| 9.0500 | -0.0067839  |
| 9.1000 | -0.0019622  |
| 9.1500 | 0.0024129   |
| 9.2000 | -0.0020723  |
| 9.2500 | -0.0035246  |
| 9.3000 | -0.0037150  |
| 9.3500 | -0.0019220  |
| 9.4000 | 0.0022554   |
| 9.4500 | 0.0042786   |
| 9.5000 | -0.0010829  |
| 9.5500 | 0.0040637   |
| 9.6000 | -0.00069420 |
| 9.6500 | 0.0077156   |
| 9.7000 | 0.0057260   |
| 9.7500 | -0.0025751  |
| 9.8000 | -0.00082894 |
| 9.8500 | 0.0085904   |
| 9.9000 | -0.0011795  |
| 9.9500 | -0.0028610  |
| 10.000 | 0.0015803   |
| 10.050 | 0.00013740  |
| 10.100 | -0.0058049  |
| 10.150 | -0.00066639 |
| 10.200 | -3.2264e-05 |
| 10.250 | 0.00020117  |
| 10.300 | 0.0042194   |

10.350 -0.0011281

### **S6.3. b-CFA**

1.8500 0.055294  
1.9000 0.045488  
1.9500 0.034782  
2.0000 0.0098723  
2.0500 -0.022639  
2.1000 -0.046704  
2.1500 -0.084367  
2.2000 -0.10673  
2.2500 -0.12529  
2.3000 -0.13152  
2.3500 -0.13915  
2.4000 -0.13731  
2.4500 -0.13014  
2.5000 -0.12304  
2.5500 -0.10717  
2.6000 -0.079827  
2.6500 -0.046681  
2.7000 -0.0077393  
2.7500 0.040292  
2.8000 0.069177  
2.8500 0.10603  
2.9000 0.12526  
2.9500 0.13211  
3.0000 0.13459  
3.0500 0.12709  
3.1000 0.11370  
3.1500 0.092474  
3.2000 0.073594  
3.2500 0.057504  
3.3000 0.038009  
3.3500 0.023599  
3.4000 0.014429  
3.4500 -0.0021692  
3.5000 -0.0096137  
3.5500 -0.020960  
3.6000 -0.027007  
3.6500 -0.042476  
3.7000 -0.053176  
3.7500 -0.058723  
3.8000 -0.069619  
3.8500 -0.070449  
3.9000 -0.071783  
3.9500 -0.071356  
4.0000 -0.064191  
4.0500 -0.055459  
4.1000 -0.049325  
4.1500 -0.040262  
4.2000 -0.027181  
4.2500 -0.014592  
4.3000 0.0013122

|        |             |
|--------|-------------|
| 4.3500 | 0.014292    |
| 4.4000 | 0.020504    |
| 4.4500 | 0.032097    |
| 4.5000 | 0.034414    |
| 4.5500 | 0.028020    |
| 4.6000 | 0.026420    |
| 4.6500 | 0.025415    |
| 4.7000 | 0.028423    |
| 4.7500 | 0.028181    |
| 4.8000 | 0.024155    |
| 4.8500 | 0.026245    |
| 4.9000 | 0.025492    |
| 4.9500 | 0.024344    |
| 5.0000 | 0.024402    |
| 5.0500 | 0.020943    |
| 5.1000 | 0.020325    |
| 5.1500 | 0.018006    |
| 5.2000 | 0.0090517   |
| 5.2500 | 0.010528    |
| 5.3000 | 0.0034348   |
| 5.3500 | -0.00017450 |
| 5.4000 | -0.0049835  |
| 5.4500 | -0.014468   |
| 5.5000 | -0.021375   |
| 5.5500 | -0.024426   |
| 5.6000 | -0.027348   |
| 5.6500 | -0.035690   |
| 5.7000 | -0.031816   |
| 5.7500 | -0.031670   |
| 5.8000 | -0.035404   |
| 5.8500 | -0.028858   |
| 5.9000 | -0.024719   |
| 5.9500 | -0.015268   |
| 6.0000 | -0.0098128  |
| 6.0500 | -0.0052029  |
| 6.1000 | -0.0038968  |
| 6.1500 | 0.010025    |
| 6.2000 | 0.026080    |
| 6.2500 | 0.026051    |
| 6.3000 | 0.025032    |
| 6.3500 | 0.019822    |
| 6.4000 | 0.012778    |
| 6.4500 | 0.013500    |
| 6.5000 | 0.011426    |
| 6.5500 | 0.010968    |
| 6.6000 | 0.0093476   |
| 6.6500 | 0.0072522   |
| 6.7000 | 0.0041272   |
| 6.7500 | -0.0014032  |
| 6.8000 | -0.0039464  |
| 6.8500 | -0.0053356  |
| 6.9000 | -0.0058731  |
| 6.9500 | -0.0049939  |

|        |             |
|--------|-------------|
| 7.0000 | -0.00056484 |
| 7.0500 | 0.00078407  |
| 7.1000 | -0.0035902  |
| 7.1500 | -0.0030624  |
| 7.2000 | -0.0084718  |
| 7.2500 | -0.0081577  |
| 7.3000 | -0.0044432  |
| 7.3500 | -4.9402e-06 |
| 7.4000 | -0.0034127  |
| 7.4500 | -0.0058963  |
| 7.5000 | -0.0027771  |
| 7.5500 | -0.0038444  |
| 7.6000 | 0.00092703  |
| 7.6500 | 0.0042312   |
| 7.7000 | 0.0026004   |
| 7.7500 | 0.0033344   |
| 7.8000 | 0.0046612   |
| 7.8500 | 0.0033483   |
| 7.9000 | 0.00034855  |
| 7.9500 | 0.0021676   |
| 8.0000 | 0.0051520   |
| 8.0500 | 0.0040120   |
| 8.1000 | 0.0038615   |
| 8.1500 | 0.0023710   |
| 8.2000 | -0.0013863  |
| 8.2500 | -0.0050451  |
| 8.3000 | -0.0017407  |
| 8.3500 | 0.0010478   |
| 8.4000 | 0.0010148   |
| 8.4500 | -0.0016639  |
| 8.5000 | -0.0025777  |
| 8.5500 | -0.0029966  |
| 8.6000 | -0.0055001  |
| 8.6500 | -0.0036448  |
| 8.7000 | -0.0033697  |
| 8.7500 | -0.0022299  |
| 8.8000 | 0.00028302  |
| 8.8500 | 0.0044875   |
| 8.9000 | 0.00095468  |
| 8.9500 | 0.0028823   |
| 9.0000 | 0.0026867   |
| 9.0500 | -0.00051919 |
| 9.1000 | 0.00052932  |
| 9.1500 | 0.0034856   |
| 9.2000 | 0.0017003   |
| 9.2500 | -0.0028868  |
| 9.3000 | -0.0010292  |
| 9.3500 | -0.0019470  |
| 9.4000 | -0.0021272  |
| 9.4500 | 0.00058001  |
| 9.5000 | 0.0031517   |
| 9.5500 | 0.00013389  |
| 9.6000 | 0.0026697   |

|        |             |
|--------|-------------|
| 9.6500 | 0.0022095   |
| 9.7000 | 0.0012230   |
| 9.7500 | 0.0040274   |
| 9.8000 | 0.00017275  |
| 9.8500 | -0.0015562  |
| 9.9000 | -0.00062765 |
| 9.9500 | 0.0031700   |
| 10.000 | 0.0044320   |
| 10.050 | 0.0019741   |
| 10.100 | -0.00018719 |
| 10.150 | -1.9289e-05 |
| 10.200 | 0.0044514   |
| 10.250 | -0.0012697  |
| 10.300 | -0.0032032  |
| 10.350 | -0.0017660  |
| 10.400 | -0.0011156  |
| 10.450 | -0.0052439  |
| 10.500 | -0.0032437  |
| 10.550 | -0.0028464  |
| 10.600 | -0.0011979  |
| 10.650 | 0.00064316  |
| 10.700 | -0.0057424  |
| 10.750 | -0.00088826 |
| 10.800 | -0.0033682  |
| 10.850 | -0.00034226 |
| 10.900 | -0.0031169  |
| 10.950 | 0.0040266   |
| 11.000 | -0.0024539  |
| 11.050 | 0.00031862  |
| 11.100 | 0.0045586   |
| 11.150 | 0.0017167   |
| 11.200 | 0.0017421   |
| 11.250 | 6.4417e-05  |

#### S6.4. Gd-HAp

|           |                 |
|-----------|-----------------|
| 2.0000000 | -0.69223473E-01 |
| 2.0500000 | -0.90963878E-01 |
| 2.1000000 | -0.11222169     |
| 2.1500000 | -0.13029805     |
| 2.2000000 | -0.14299038     |
| 2.2500000 | -0.15050603     |
| 2.3000000 | -0.15347093     |
| 2.3500000 | -0.15069914     |
| 2.4000000 | -0.14409002     |
| 2.4500000 | -0.13248524     |
| 2.5000000 | -0.11665278     |
| 2.5500000 | -0.94847726E-01 |
| 2.6000000 | -0.67317191E-01 |
| 2.6500000 | -0.36980764E-01 |
| 2.7000000 | -0.25144367E-02 |
| 2.7500000 | 0.31933213E-01  |
| 2.8000000 | 0.63341922E-01  |
| 2.8500000 | 0.90570754E-01  |

|           |                 |
|-----------|-----------------|
| 2.9000000 | 0.11102141      |
| 2.9500000 | 0.12385464      |
| 3.0000000 | 0.12803103      |
| 3.0500000 | 0.12426942      |
| 3.1000000 | 0.11652133      |
| 3.1500000 | 0.10433383      |
| 3.2000000 | 0.88850081E-01  |
| 3.2500000 | 0.73207659E-01  |
| 3.3000000 | 0.56683966E-01  |
| 3.3500000 | 0.41661626E-01  |
| 3.4000000 | 0.26451554E-01  |
| 3.4500000 | 0.95455087E-02  |
| 3.5000000 | -0.27301179E-02 |
| 3.5500000 | -0.15865058E-01 |
| 3.6000000 | -0.29582133E-01 |
| 3.6500000 | -0.38894468E-01 |
| 3.7000000 | -0.48234915E-01 |
| 3.7500000 | -0.56978439E-01 |
| 3.8000000 | -0.61231164E-01 |
| 3.8500000 | -0.65866069E-01 |
| 3.9000000 | -0.67047212E-01 |
| 3.9500000 | -0.65700198E-01 |
| 4.0000000 | -0.61942563E-01 |
| 4.0500000 | -0.55392598E-01 |
| 4.1000000 | -0.47162418E-01 |
| 4.1500000 | -0.37319818E-01 |
| 4.2000000 | -0.21042362E-01 |
| 4.2500000 | -0.10297150E-01 |
| 4.3000000 | 0.19793483E-02  |
| 4.3500000 | 0.92211571E-02  |
| 4.4000000 | 0.14934115E-01  |
| 4.4500000 | 0.20467405E-01  |
| 4.5000000 | 0.22482400E-01  |
| 4.5500000 | 0.24081163E-01  |
| 4.6000000 | 0.24496661E-01  |
| 4.6500000 | 0.23658561E-01  |
| 4.7000000 | 0.24259678E-01  |
| 4.7500000 | 0.24071356E-01  |
| 4.8000000 | 0.23816160E-01  |
| 4.8500000 | 0.24768342E-01  |
| 4.9000000 | 0.24280241E-01  |
| 4.9500000 | 0.24692931E-01  |
| 5.0000000 | 0.24108289E-01  |
| 5.0500000 | 0.22746978E-01  |
| 5.1000000 | 0.20880776E-01  |
| 5.1500000 | 0.16900145E-01  |
| 5.2000000 | 0.14686710E-01  |
| 5.2500000 | 0.10074007E-01  |
| 5.3000000 | 0.51845507E-02  |
| 5.3500000 | 0.83507962E-03  |
| 5.4000000 | -0.52462895E-02 |
| 5.4500000 | -0.10085122E-01 |
| 5.5000000 | -0.15172909E-01 |

|           |                 |
|-----------|-----------------|
| 5.5500000 | -0.20113215E-01 |
| 5.6000000 | -0.23207584E-01 |
| 5.6500000 | -0.25589451E-01 |
| 5.7000000 | -0.27676143E-01 |
| 5.7500000 | -0.27571199E-01 |
| 5.8000000 | -0.25967297E-01 |
| 5.8500000 | -0.23189421E-01 |
| 5.9000000 | -0.20154334E-01 |
| 5.9500000 | -0.15942436E-01 |
| 6.0000000 | -0.11327828E-01 |
| 6.0500000 | -0.55817884E-02 |
| 6.1000000 | 0.13568477E-04  |
| 6.1500000 | 0.60612415E-02  |
| 6.2000000 | 0.12817814E-01  |
| 6.2500000 | 0.18058811E-01  |
| 6.3000000 | 0.18388897E-01  |
| 6.3500000 | 0.17070052E-01  |
| 6.4000000 | 0.15277724E-01  |
| 6.4500000 | 0.14064656E-01  |
| 6.5000000 | 0.13140331E-01  |
| 6.5500000 | 0.10646431E-01  |
| 6.6000000 | 0.80629917E-02  |
| 6.6500000 | 0.52200755E-02  |
| 6.7000000 | 0.12947766E-02  |
| 6.7500000 | -0.89125491E-03 |
| 6.8000000 | -0.21578804E-02 |
| 6.8500000 | -0.28252132E-02 |
| 6.9000000 | -0.33600754E-02 |
| 6.9500000 | -0.34323520E-02 |
| 7.0000000 | -0.34259514E-02 |
| 7.0500000 | -0.19394824E-02 |
| 7.1000000 | -0.25194811E-02 |
| 7.1500000 | -0.37852679E-02 |
| 7.2000000 | -0.40625077E-02 |
| 7.2500000 | -0.45769494E-02 |
| 7.3000000 | -0.41533948E-02 |
| 7.3500000 | -0.41370120E-02 |
| 7.4000000 | -0.40539100E-02 |
| 7.4500000 | -0.35118605E-02 |
| 7.5000000 | -0.27744651E-02 |
| 7.5500000 | -0.17069102E-02 |
| 7.6000000 | -0.16715956E-03 |
| 7.6500000 | 0.12116148E-02  |
| 7.7000000 | 0.21483912E-02  |
| 7.7500000 | 0.22224893E-02  |
| 7.8000000 | 0.22639756E-02  |
| 7.8500000 | 0.34627276E-02  |
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| 8.1000000 | 0.25300955E-02  |
| 8.1500000 | 0.18741588E-02  |

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| 8.2000000 | 0.21442005E-02  |
| 8.2500000 | 0.24218718E-05  |
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| 8.9000000 | -0.32613462E-03 |
| 8.9500000 | -0.11954666E-02 |
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| 9.2500000 | -0.10703796E-02 |
| 9.3000000 | -0.22886829E-03 |
| 9.3500000 | -0.99732186E-03 |
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| 9.4500000 | 0.25332659E-03  |
| 9.5000000 | -0.78896288E-04 |
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| 9.8500000 | 0.10282878E-02  |
| 9.9000000 | 0.87560984E-03  |
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| 10.150000 | -0.17128923E-03 |
| 10.200000 | -0.11570959E-03 |
| 10.250000 | 0.84975845E-04  |
| 10.300000 | -0.86972545E-03 |
| 10.350000 | -0.21550154E-03 |
| 10.400000 | -0.26153163E-03 |
| 10.450000 | -0.87588456E-03 |
| 10.500000 | -0.72879614E-03 |
| 10.550000 | -0.30766616E-03 |
| 10.600000 | -0.11759098E-02 |
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| 10.750000 | -0.92908955E-04 |
| 10.800000 | -0.16572902E-03 |

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| 10.900000 | 0.33623659E-03  |
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| 11.050000 | 0.21097767E-03  |
| 11.100000 | 0.55102832E-03  |
| 11.150000 | 0.99590879E-03  |
| 11.200000 | 0.55501167E-03  |
| 11.250000 | 0.75131829E-03  |
| 11.300000 | 0.56379637E-03  |
| 11.350000 | 0.47723423E-03  |
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| 11.600000 | -0.38694691E-03 |
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| 12.400000 | 0.44113712E-03  |
| 12.450000 | 0.43501198E-03  |
| 12.500000 | -0.29941883E-03 |
| 12.550000 | 0.24382490E-03  |
| 12.600000 | -0.16734788E-03 |
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### S6.5. Gd,Y-HAp

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| 2.3500000 | -0.15179389     |
| 2.4000000 | -0.14429879     |
| 2.4500000 | -0.13217413     |
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| 2.8000000 | 0.68210096E-01  |
| 2.8500000 | 0.93388929E-01  |
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| 3.0000000 | 0.13280512      |
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| 3.1500000 | 0.10874770      |
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| 3.3000000 | 0.55528097E-01  |
| 3.3500000 | 0.37607725E-01  |
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| 3.7000000 | -0.54412296E-01 |
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| 3.8500000 | -0.68145238E-01 |
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| 4.3000000 | 0.17244249E-02  |
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| 4.4500000 | 0.20603890E-01  |
| 4.5000000 | 0.24414630E-01  |
| 4.5500000 | 0.25790793E-01  |
| 4.6000000 | 0.27117417E-01  |
| 4.6500000 | 0.27363865E-01  |
| 4.7000000 | 0.27700251E-01  |
| 4.7500000 | 0.26895510E-01  |
| 4.8000000 | 0.27696334E-01  |
| 4.8500000 | 0.27885388E-01  |
| 4.9000000 | 0.25920467E-01  |
| 4.9500000 | 0.25847715E-01  |
| 5.0000000 | 0.23215836E-01  |
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| 5.1500000 | 0.13863104E-01  |
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| 5.7500000 | -0.26102227E-01 |
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| 5.8500000 | -0.21678116E-01 |
| 5.9000000 | -0.18457936E-01 |
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| 7.7500000 | 0.24310360E-02  |
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| 7.9500000 | 0.34587266E-02  |
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| 8.1000000 | 0.27562230E-02  |
| 8.1500000 | 0.20347793E-02  |
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| 10.500000 | -0.10161113E-02 |

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| 10.550000 | -0.16930157E-03 |
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| 10.800000 | -0.74294522E-03 |
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