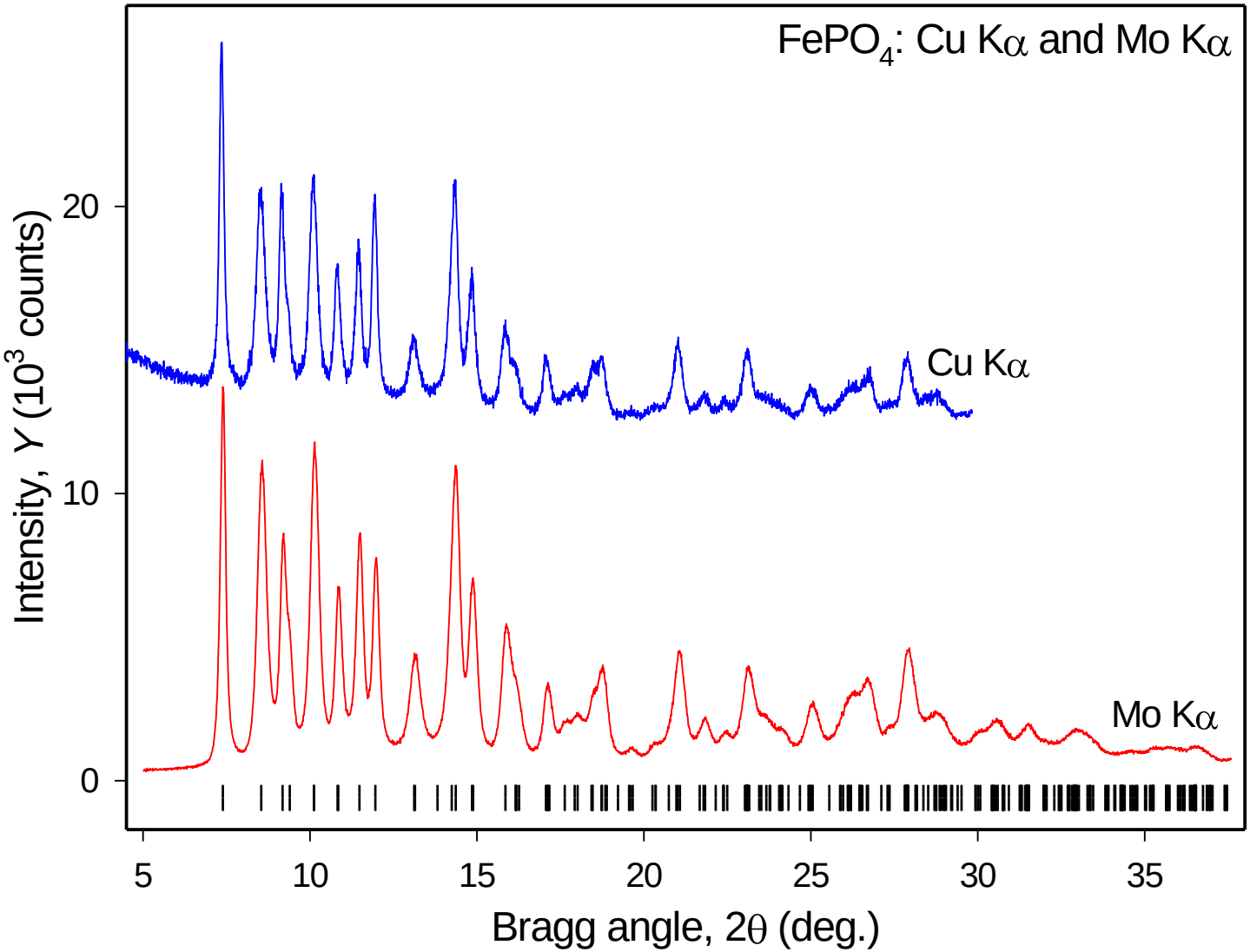
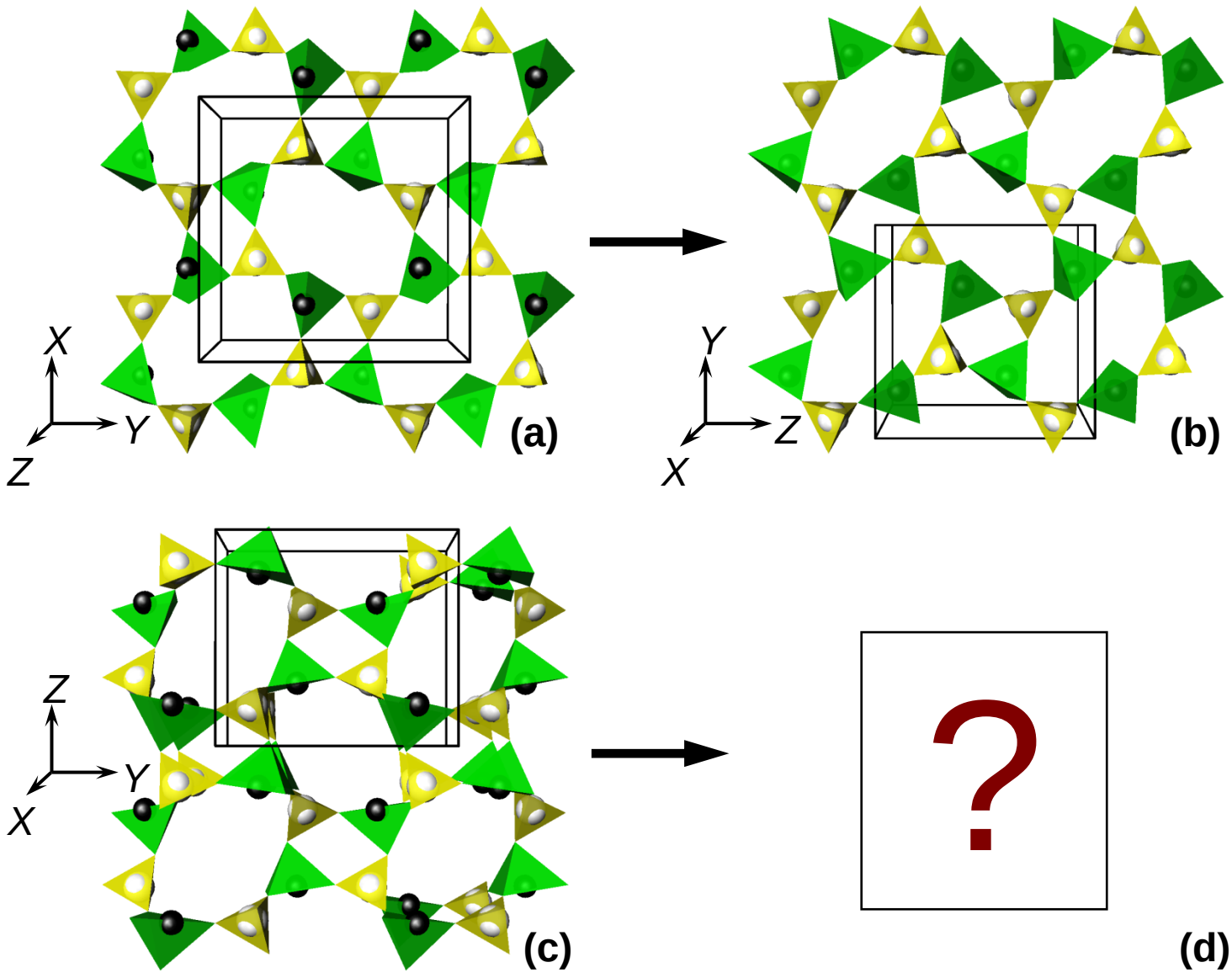
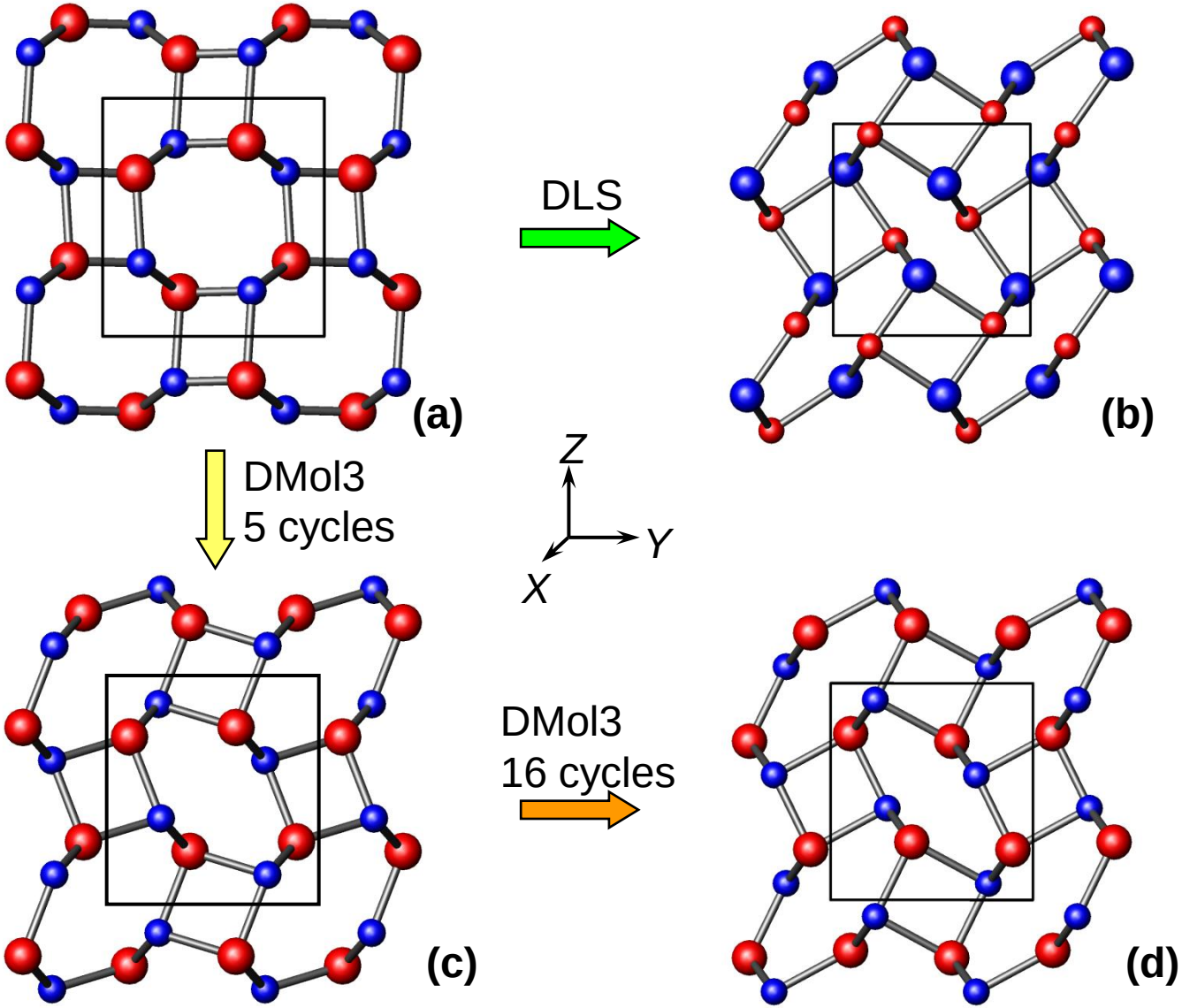
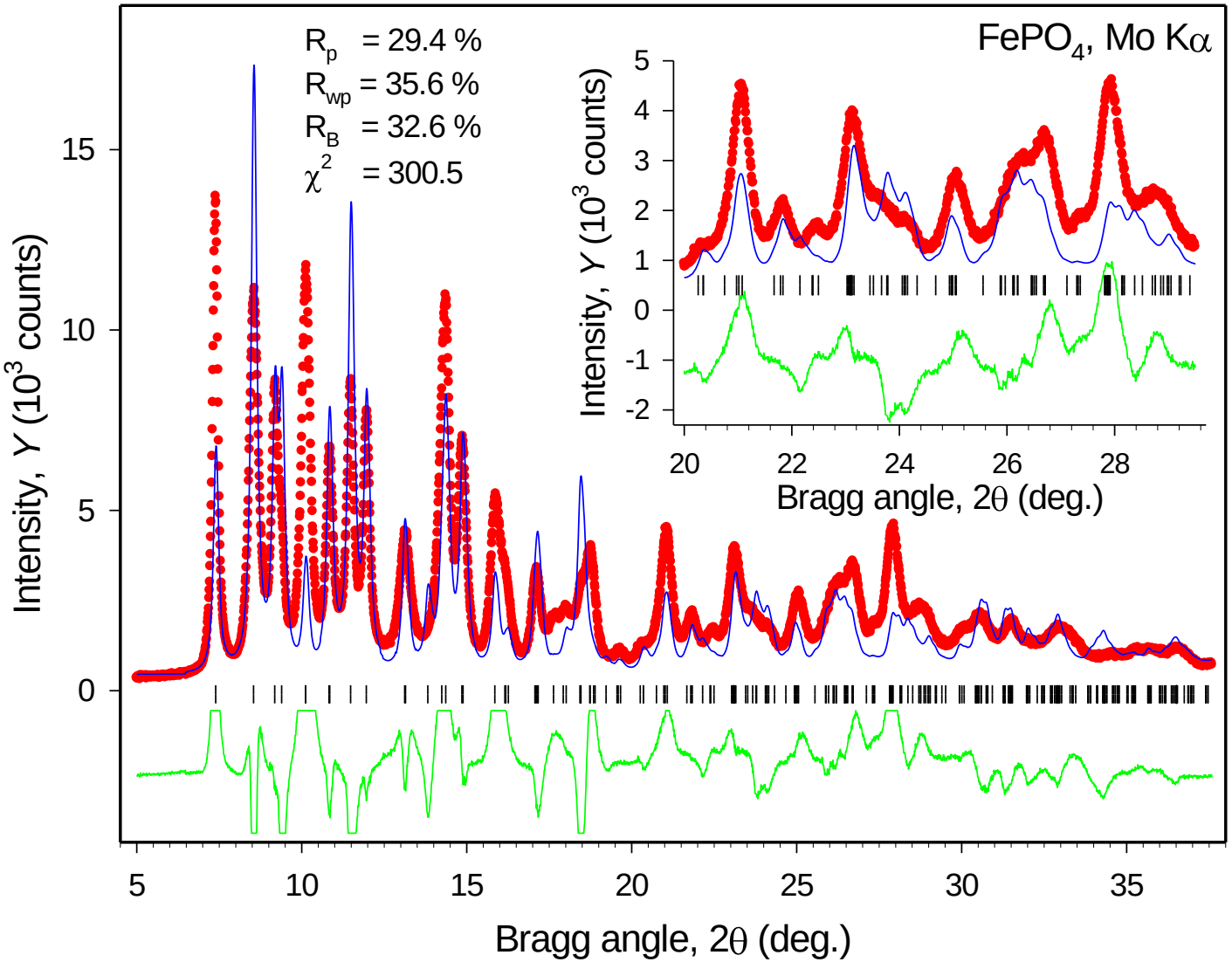
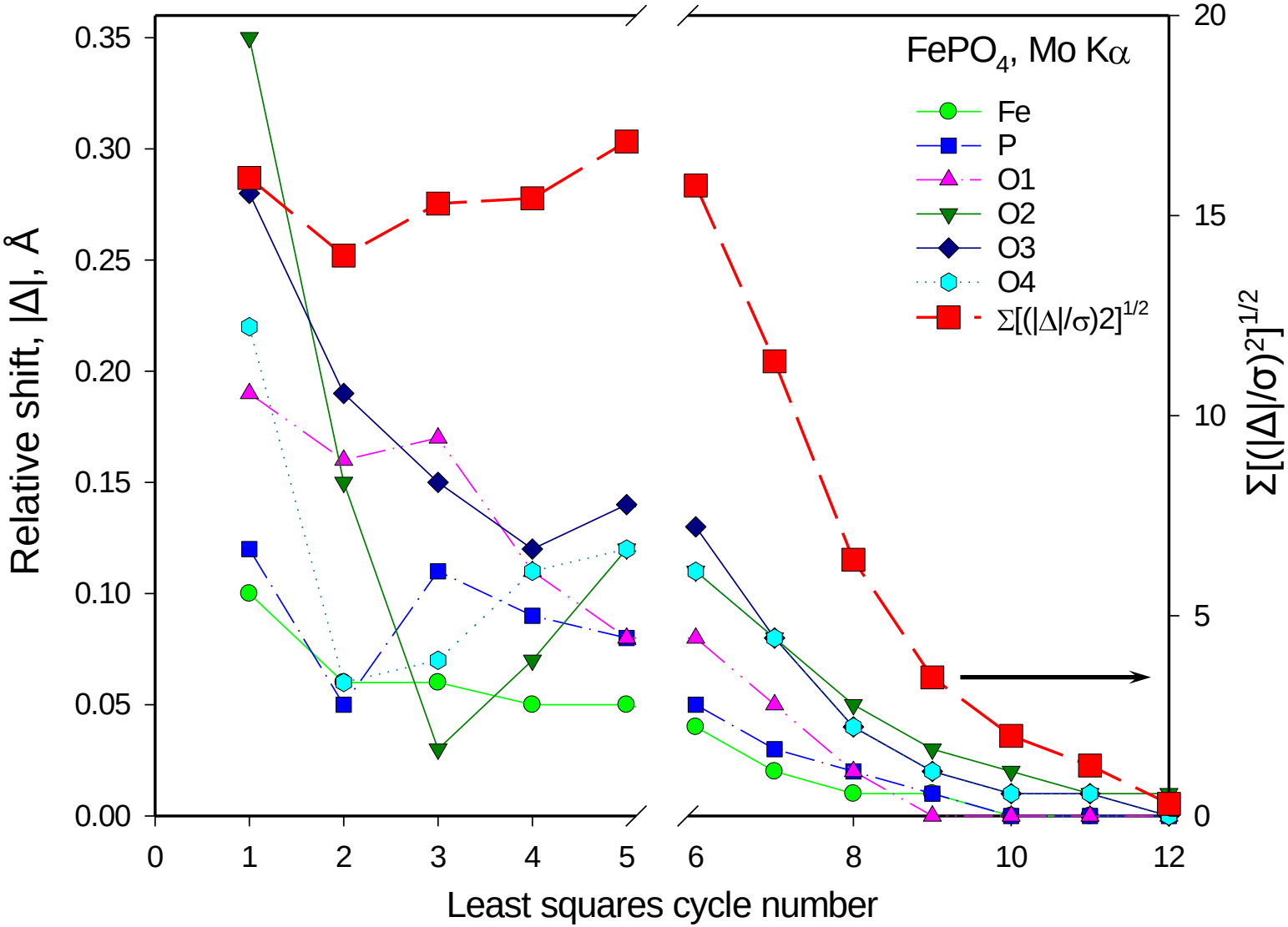
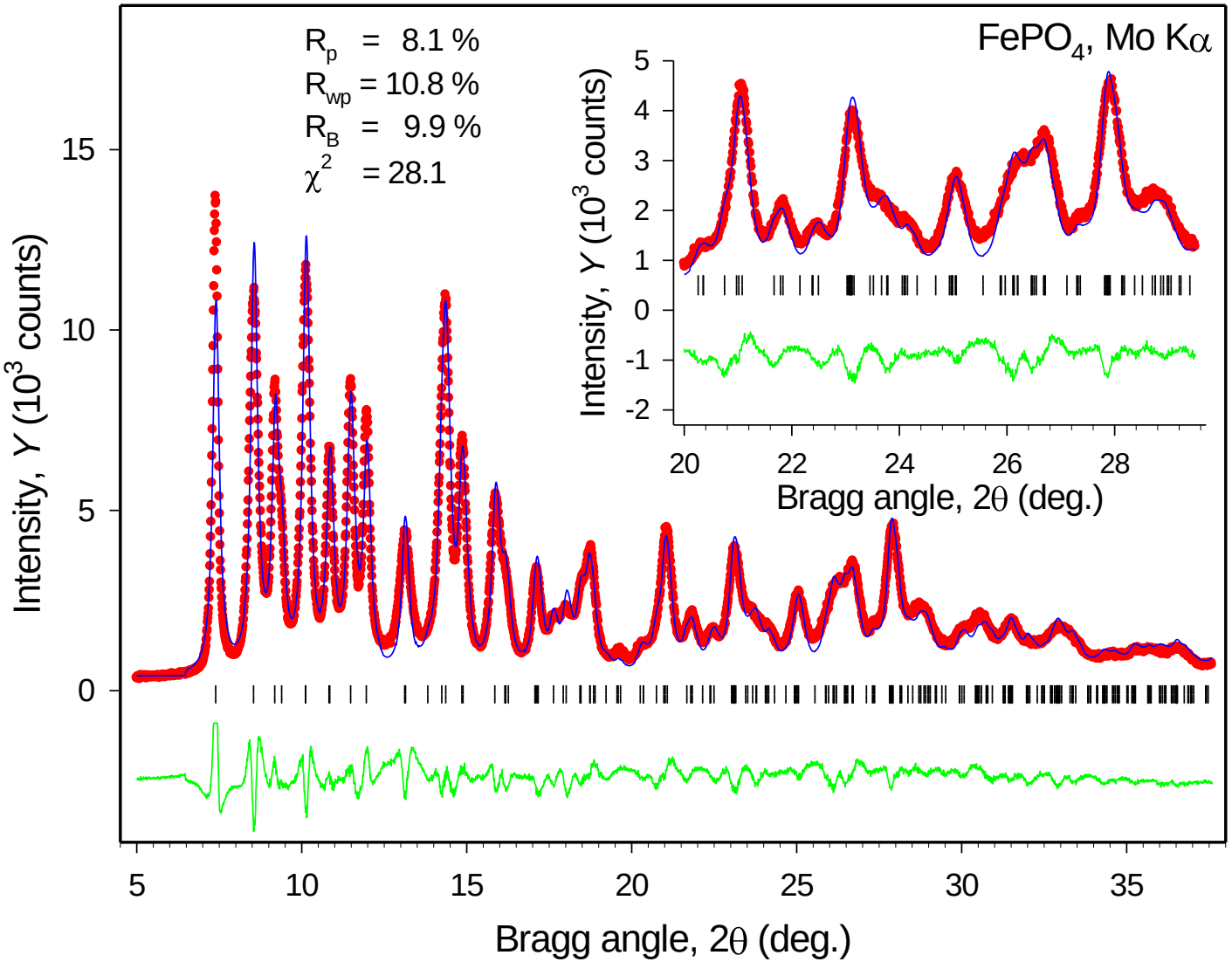

FePO4: Cu Kα and Mo Kα
Cu Kα
Mo Kα
Intensity, Y (10^3 counts)
0
10
20
5
10
15
20
25
30
35
Bragg angle, 2θ (deg.)

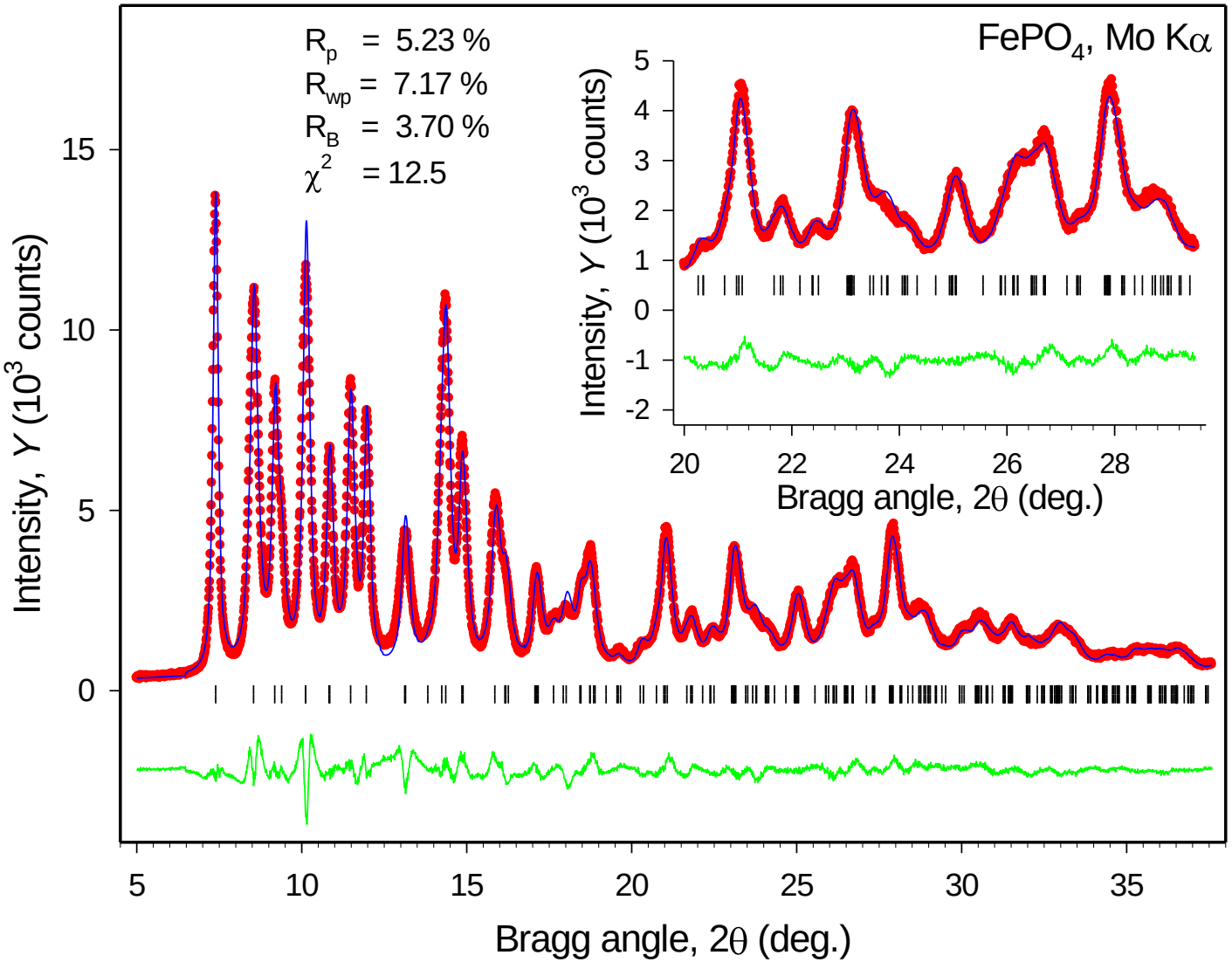

X
Y
Z
(a)
Y
Z
X
(b)
Z
Y
X
(c)
?
(d)

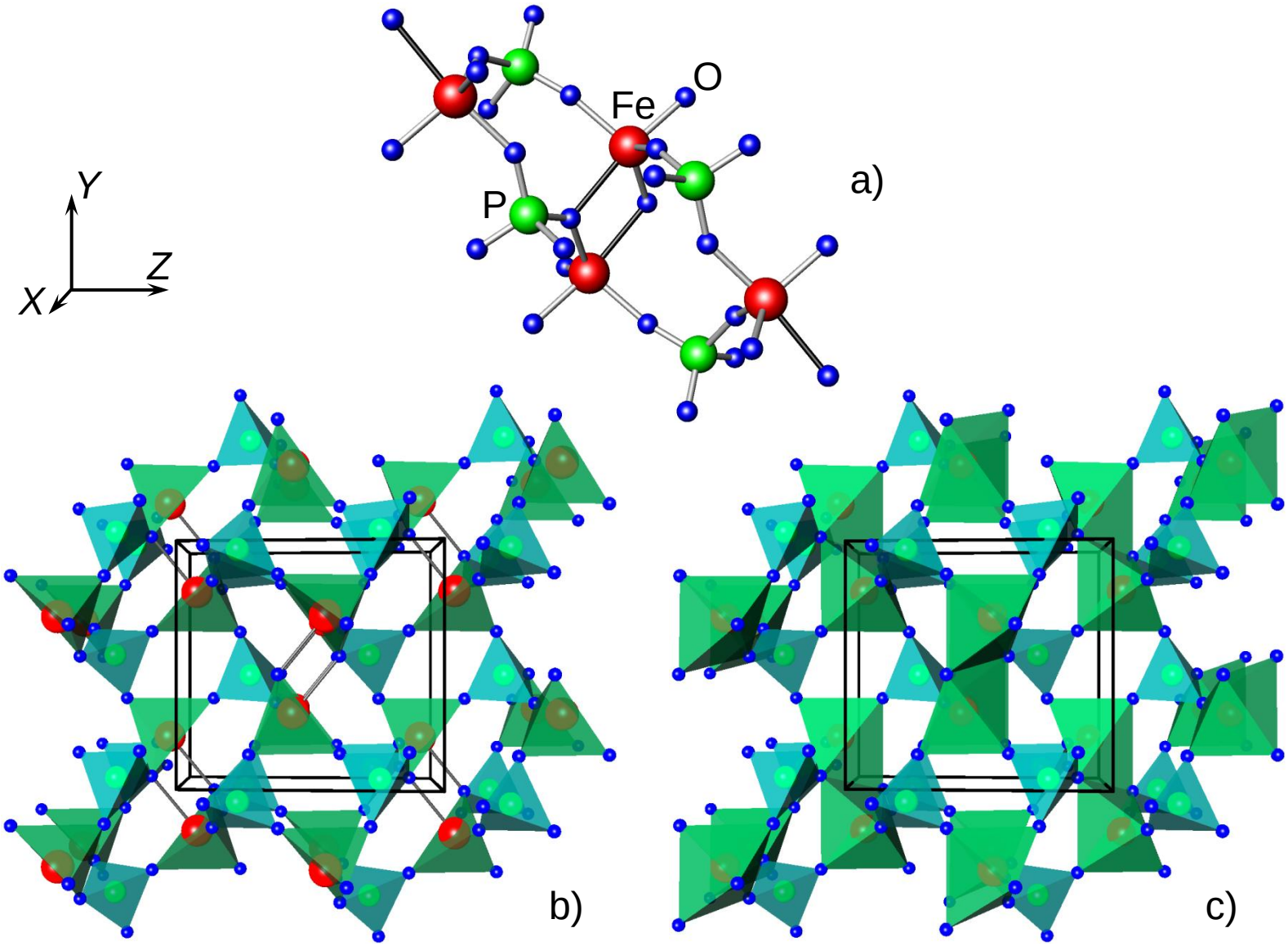

DLS
(a)
(b)
DMol3
5 cycles
Z
Y
X
DMol3
16 cycles
(c)
(d)


R_p = 29.4 %
R_{wp} = 35.6 %
R_B = 32.6 %
χ^2 = 300.5
$FePO_4$, Mo Kα
Intensity, Y (10^3 counts)
Bragg angle, 2θ (deg.)
0
5
10
15
20
22
24
26
28
-2
-1
1
2
3
4
25
30
35


FePO4, Mo Kα
Fe
P
O1
O2
O3
O4
Σ[(|Δ|/σ)2]1/2
Relative shift, |Δ|, Å
Σ[(|Δ|/σ)2]1/2
Least squares cycle number
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
1
2
3
4
5
6
8
10
12
20
15
10
5
0


R_p = 8.1 %
R_{wp} = 10.8 %
R_B = 9.9 %
χ^2 = 28.1
$FePO_4$, Mo Kα
Intensity, Y (10^3 counts)
Bragg angle, 2θ (deg.)
0
5
10
15
20
25
30
35
-2
-1
1
2
3
4


R_p = 5.23 %
R_{wp} = 7.17 %
R_B = 3.70 %
χ^2 = 12.5
$FePO_4$, Mo Kα
Intensity, Y (10^3 counts)
Bragg angle, 2θ (deg.)
0
5
10
15
20
22
24
26
28
-2
-1
1
2
3
4
25
30
35



Ch. 24. Crystal Structure of $FePO_4$

Fig. 24.8