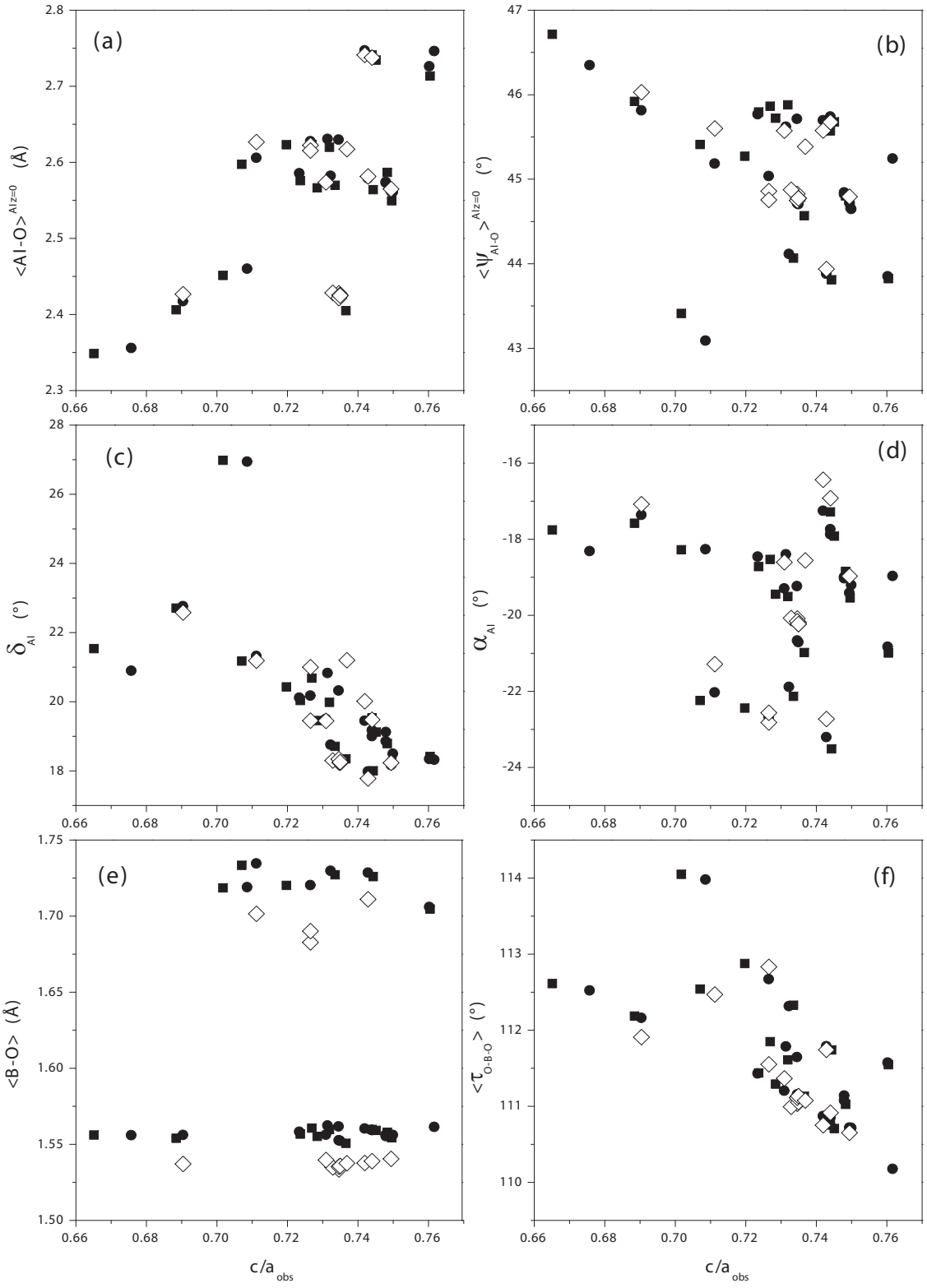


Figure 8

Correlations of observed c/a ratios with the following crystal-chemical parameters: $\langle Al\text{-}O\rangle^{Alz=0}$ (*a*), $\langle \psi_{Al\text{-}O} \rangle^{Alz=0}$ (*b*), δ_{Al} (*c*), α_{Al} (*d*), <B-O> (*e*), and $\langle \tau_{O\text{-}B\text{-}O} \rangle$ (*f*). Legend for synbols as in Figure 3.

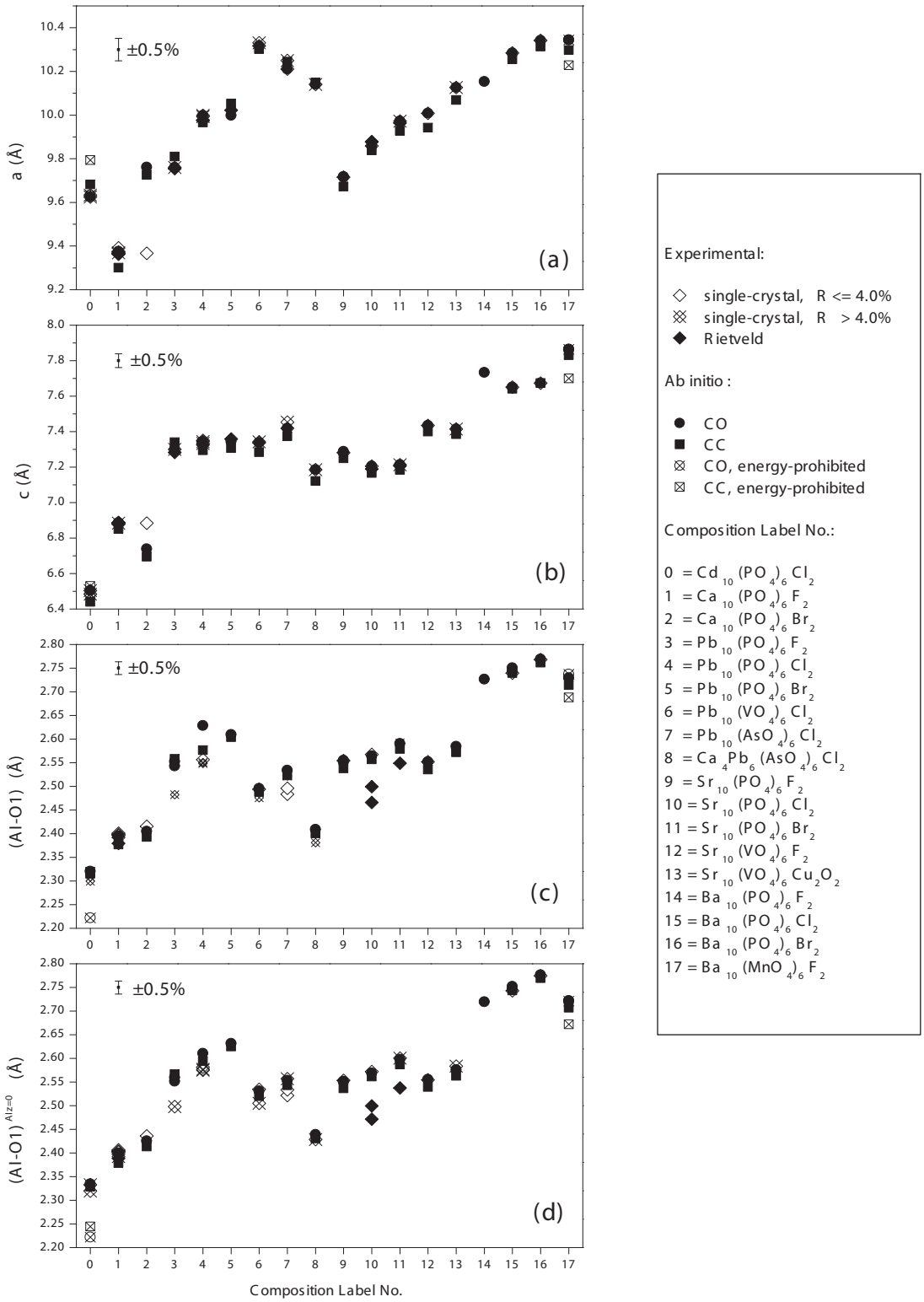
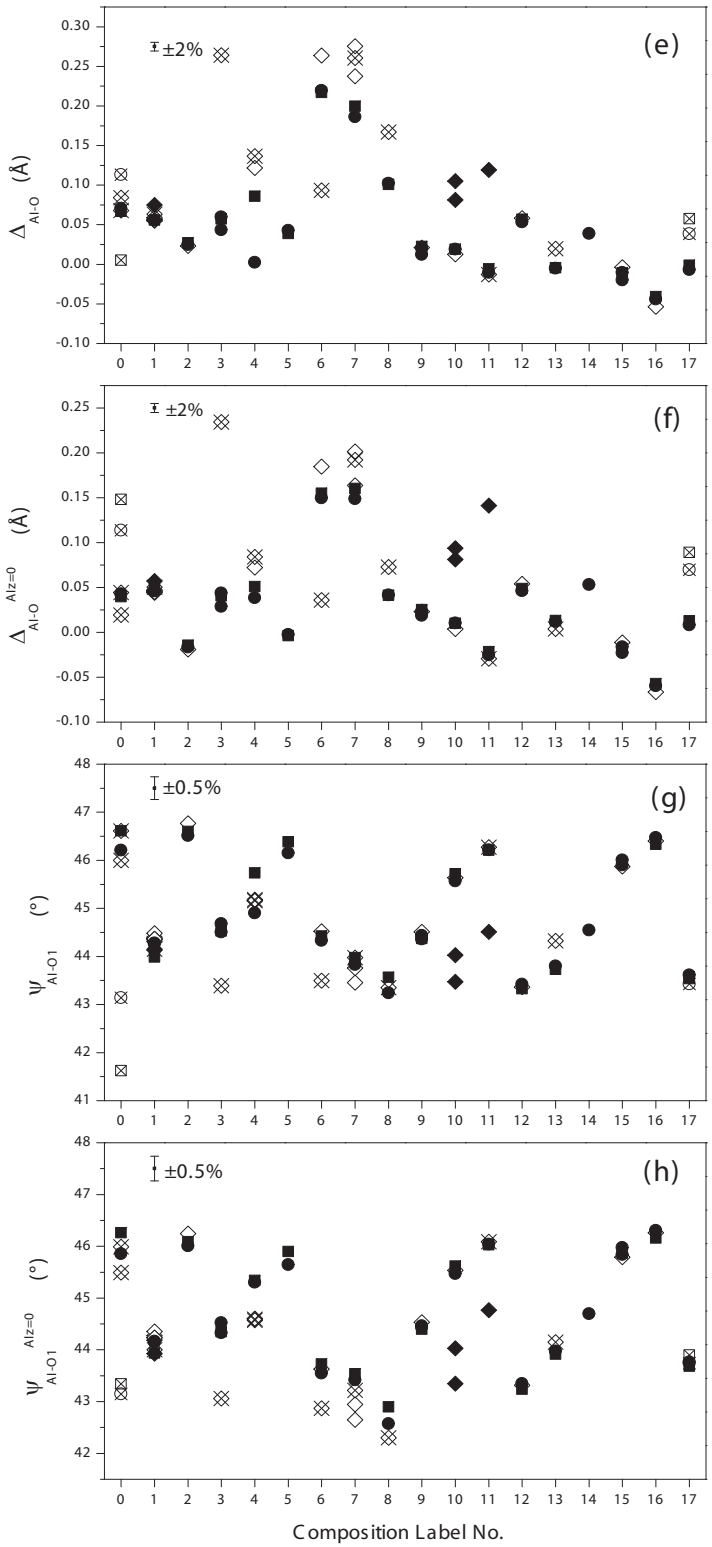


Figure 9
Comparison of experimental data with *ab initio* results.



Experimental:

- ◇ single-crystal, R <= 4.0%
- ⊠ single-crystal, R > 4.0%
- ◆ Rietveld

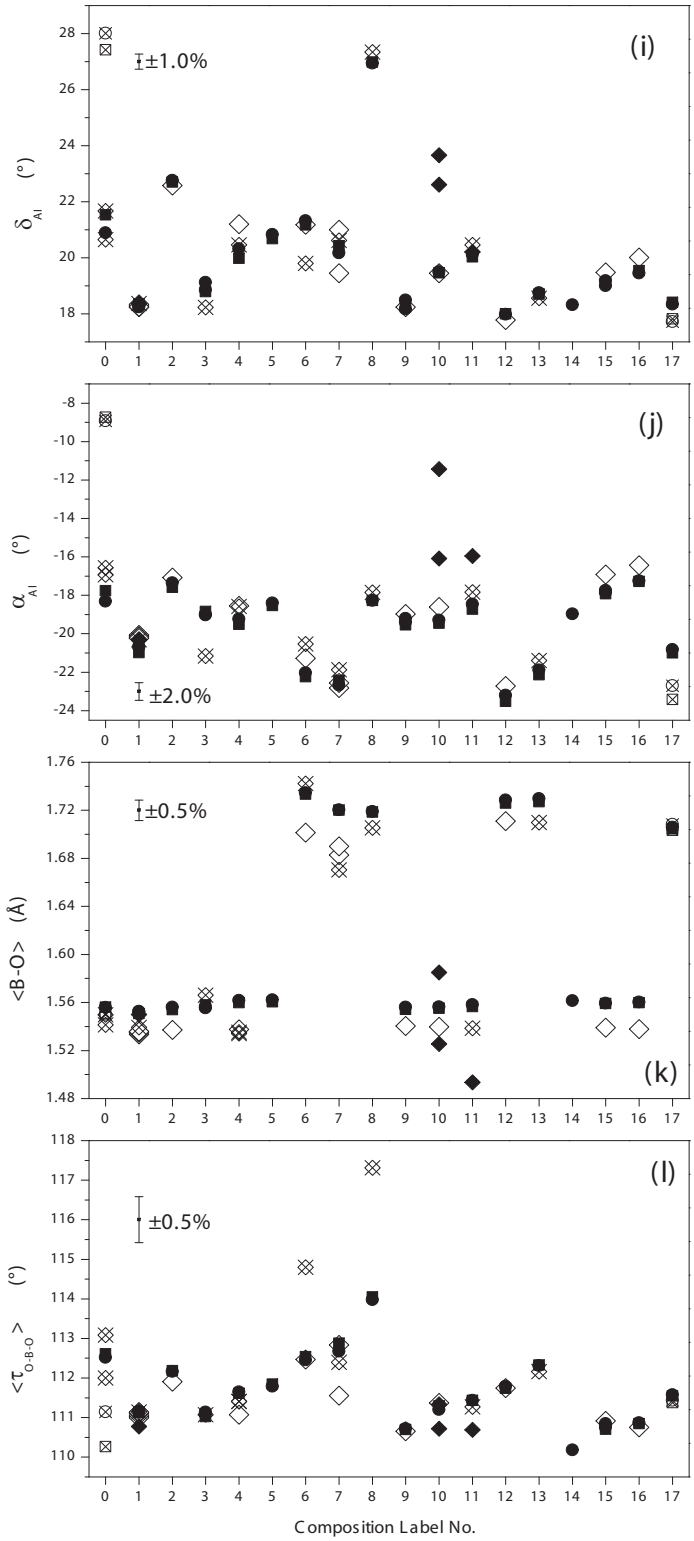
Ab initio:

- ● CO
- ■ CC
- ⊠ CO, energy-prohibited
- ⊠ CC, energy-prohibited

Composition Label No.:

0 = $Cd_{10}(PO_4)_6Cl_2$
1 = $Ca_{10}(PO_4)_6F_2$
2 = $Ca_{10}(PO_4)_6Br_2$
3 = $Pb_{10}(PO_4)_6F_2$
4 = $Pb_{10}(PO_4)_6Cl_2$
5 = $Pb_{10}(PO_4)_6Br_2$
6 = $Pb_{10}(VO_4)_6Cl_2$
7 = $Pb_{10}(AsO_4)_6Cl_2$
8 = $Ca_4Pb_6(AsO_4)_6Cl_2$
9 = $Sr_{10}(PO_4)_6F_2$
10 = $Sr_{10}(PO_4)_6Cl_2$
11 = $Sr_{10}(PO_4)_6Br_2$
12 = $Sr_{10}(VO_4)_6F_2$
13 = $Sr_{10}(VO_4)_6Cu_2O_2$
14 = $Ba_{10}(PO_4)_6F_2$
15 = $Ba_{10}(PO_4)_6Cl_2$
16 = $Ba_{10}(PO_4)_6Br_2$
17 = $Ba_{10}(MnO_4)_6F_2$

Figure 9
Continued.



Experimental:

- ◇ single-crystal, R <= 4.0%
- ⊠ single-crystal, R > 4.0%
- ◆ Rietveld

Ab initio :

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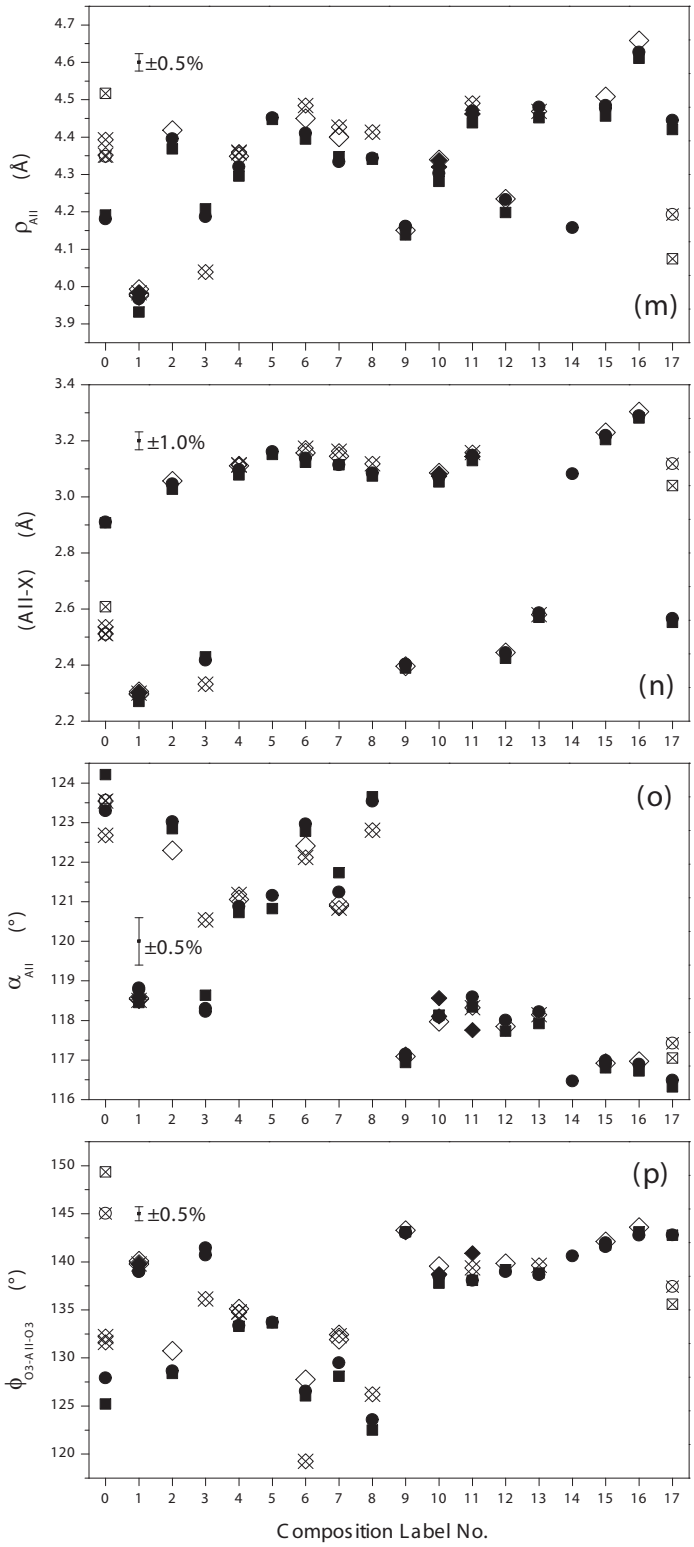
4 = $Pb_{10}(PO_4)_6Cl_2$
5 = $Pb_{10}(PO_4)_6Br_2$
6 = $Pb_{10}(VO_4)_6Cl_2$
7 = $Pb_{10}(AsO_4)_6Cl_2$
8 = $Ca_4Pb_6(AsO_4)_6Cl_2$
9 = $Sr_{10}(PO_4)_6F_2$
10 = $Sr_{10}(PO_4)_6Cl_2$
11 = $Sr_{10}(PO_4)_6Br_2$
12 = $Sr_{10}(VO_4)_6F_2$
13 = $Sr_{10}(VO_4)_6Cu_2O_2$
14 = $Ba_{10}(PO_4)_6F_2$
15 = $Ba_{10}(PO_4)_6Cl_2$
16 = $Ba_{10}(PO_4)_6Br_2$
17 = $Ba_{10}(MnO_4)_6F_2$

Figure 9
Continued.



Experimental:

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- ⊗ single-crystal, R > 4.0%
- ◆ Rietveld

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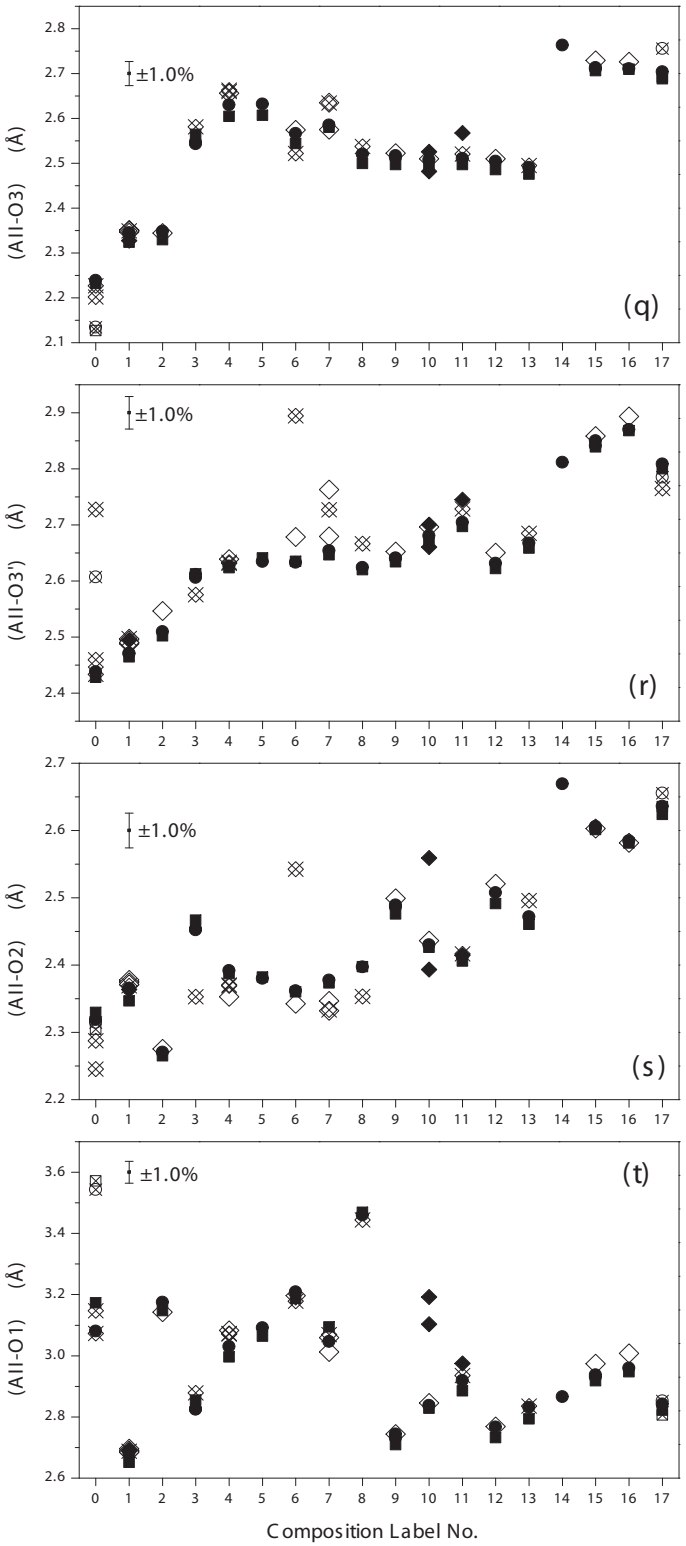
13 = $Sr_{10}(VO_4)_6Cu_2O_2$
14 = $Ba_{10}(PO_4)_6F_2$
15 = $Ba_{10}(PO_4)_6Cl_2$
16 = $Ba_{10}(PO_4)_6Br_2$
17 = $Ba_{10}(MnO_4)_6F_2$

Figure 9
Continued.



Experimental:

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15 = $Ba_{10}(PO_4)_6Cl_2$
16 = $Ba_{10}(PO_4)_6Br_2$
17 = $Ba_{10}(MnO_4)_6F_2$

Figure 9
Continued.