Perovskites and Spinels

Perovskites:

The general formula for this kind of structure is ABO_3 where A and B atoms are cations. $CaTiO_3$ is an ideal example for the perovskite structure. In $CaTiO_3$ (cubic) the oxygen anions **and** calcium cations form a cubic close packing whereas titanium cations occupy 1/4 of the octahedral holes.
Calcium is cuboctahedrally coordinated by 12 oxide ions whereas titanium is octahedrally coordinated by 6 oxide ions. In literature we can distinguish between two equivalent types of cubic unit cells (two different origins) for perovskite structure. In the first unit cell Ca is located in the centre, Ti ions on the corners and oxygen ions on the edges). In the second one Ti occupy the centre, oxygen ions the centre of each faces and Ca ions the corners of the cubic unit cell.

Application of perovskites:

1. If the B-atom is not exactly located in the centre of the octahedra holes (distortion) perovskites show high dielectric constants (e.g. $BaTiO_3$) and are thus used in capacitors.
2. Sensor and catalyst electrode in certain kinds of full cells.
3. Candidate for memory devices.

$YBa_2Cu_3O_{7-x}$:

$YBa_2Cu_3O_{7-x}$ is a famous high temperature superconductor. It has a defect perovskite structure. Y and Ba correspond with the A-atoms, Cu with the B - atoms.
The unit cell of $YBa_2Cu_3O_{7-x}$ corresponds with a triple perovskite unit cell in which some of the oxygen atoms are missing. For the Cu atoms three different coordinations result.
The electrical resistance for this compound at low temperature is exactly zero and has no interior magnetic field.

Spinels:

The spinel structure is very common in minerals and in synthetic compounds. In spinels the anions form a cubic close packed structure. Concerning the distribution of the cations we can distinguish between two kinds of spinels:

1. Normal spinel (general formula: AB_2X_4). A-atoms occupy 1/8 of the tetrahedral holes while B-atoms occupy 1/2 of the octahedral holes. (e.g. $MgAl_2O_4$).

2. Inverse spinels general formula $B[AB]O_4$. B atoms occupy 1/8 of the tetrahedral holes; B and A together occupy 1/2 of the octahedral holes (e.g. Fe_3O_4).

References:

1. A. R. West, Basic Solid State Chemistry, Second Edition, John Wiley & Sons, **1999**
2. U. Müller, Inorganic Structural Chemistry, John Wiley & Sons, **1999**