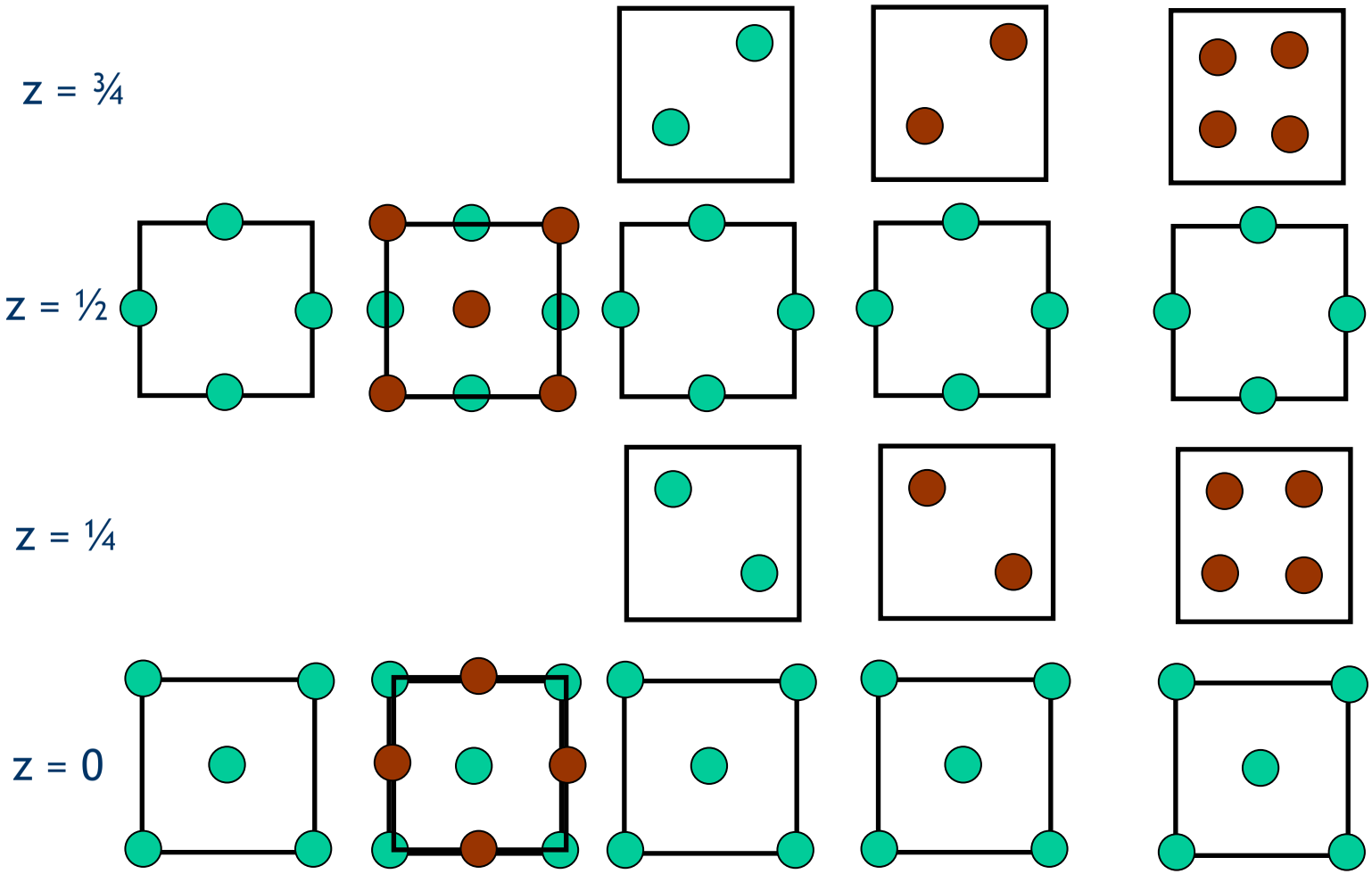
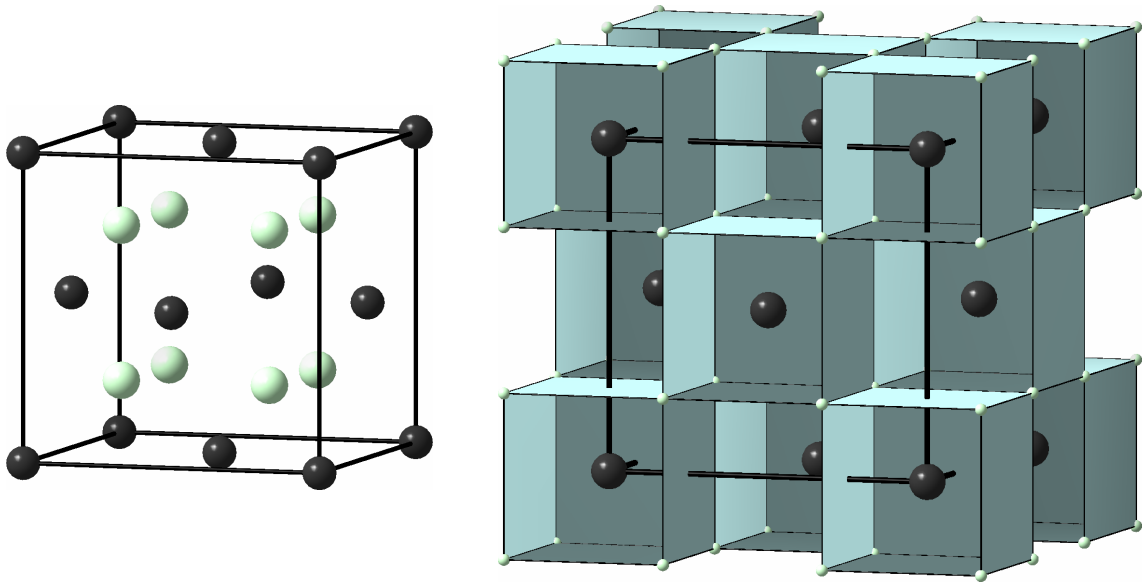
Class 7: Fluorite, pyrochlore, murataite



Class 7: Fluorite, pyrochlore, murataite

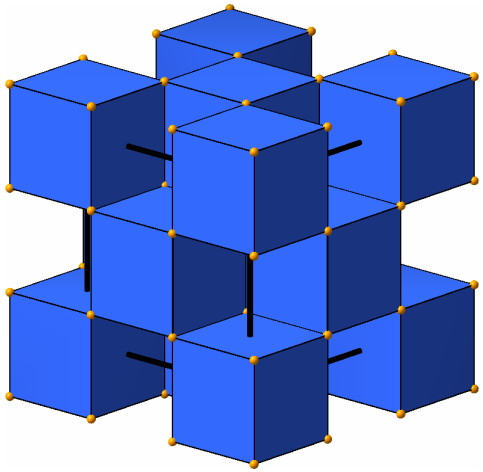


Views of the fluorite CaF_2 structure [Gerlach 1922]. Ca is 8-coordinate and F is 4-coordinate. Many oxides: UO_2, PrO_2, CeO_2, stabilized, cubic ZrO_2 and HfO_2...
Uses: CeO_2 is an oxide ion conductor. HfO_2 and ZrO_2 are important structural materials. UO_2 is "yellowcake"

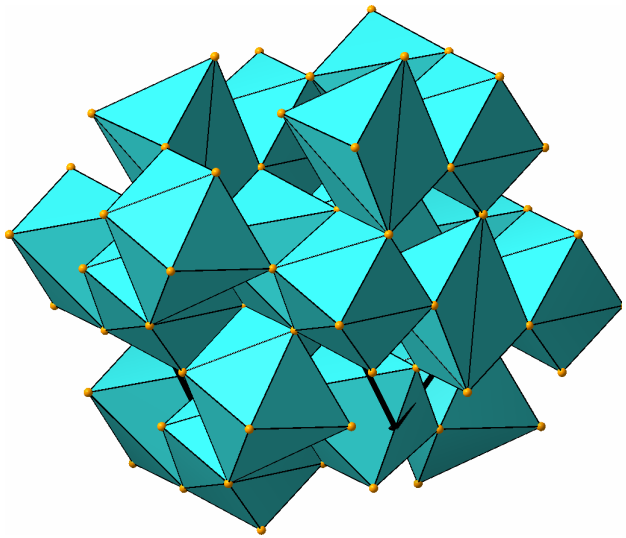
Class 7: Fluorite, pyrochlore, murataite

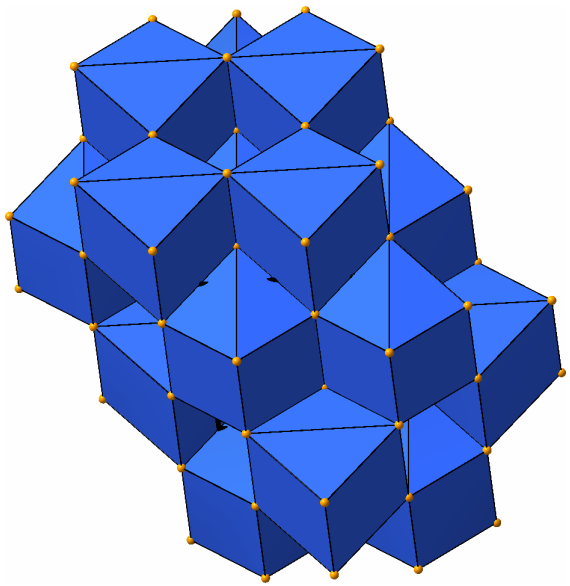
Stabilized zirconia:

cubic



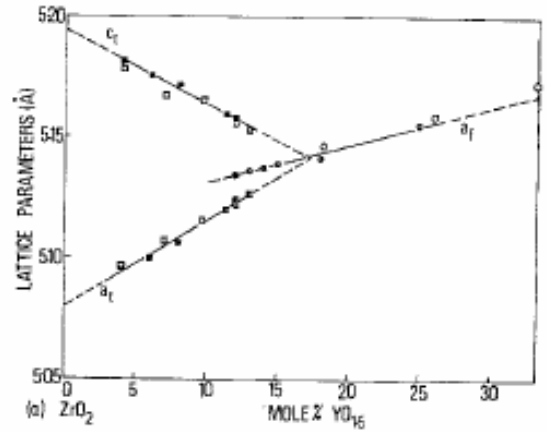
mono
baddeylite

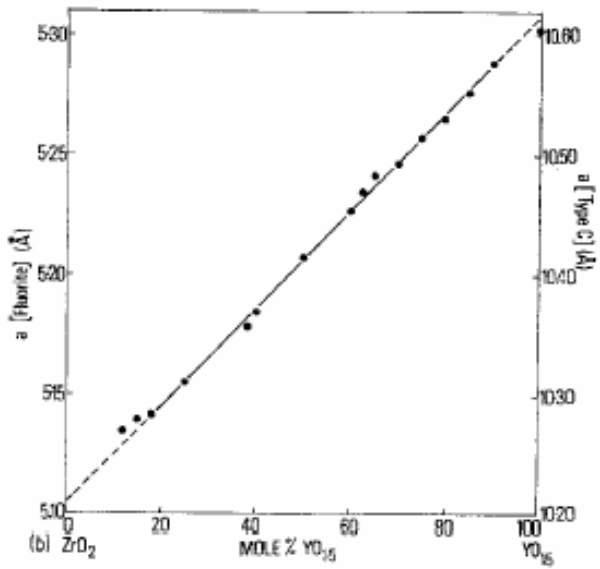




tet

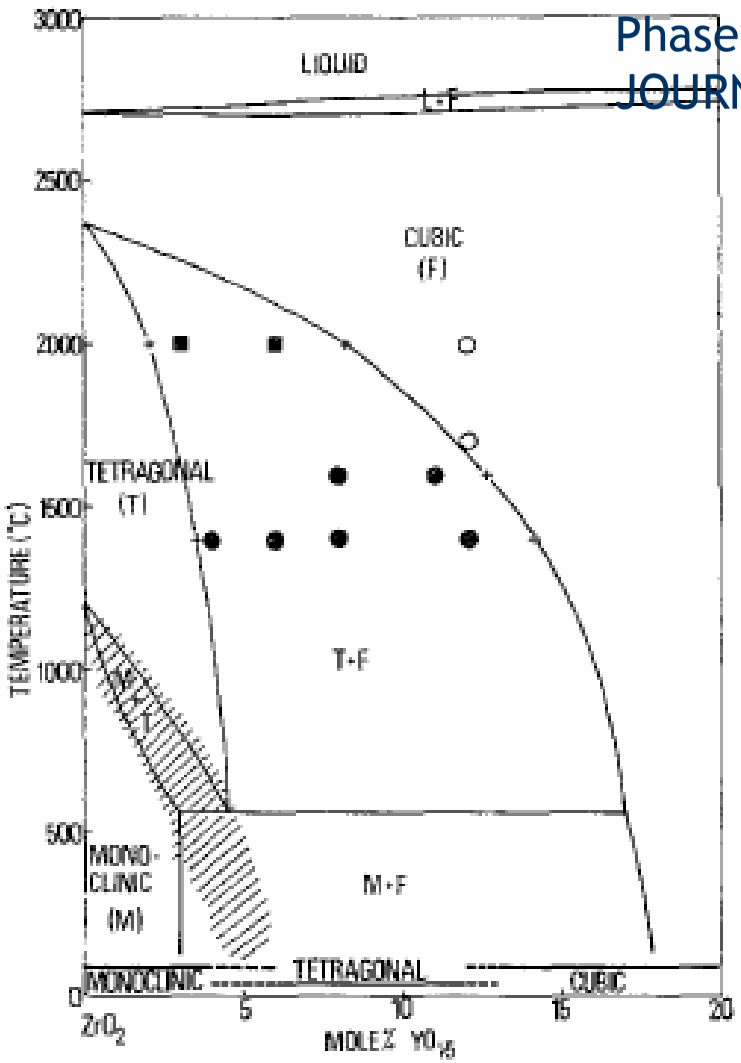
stabilization with Y_2O_3





Class 7: Fluorite, pyrochlore, murataite

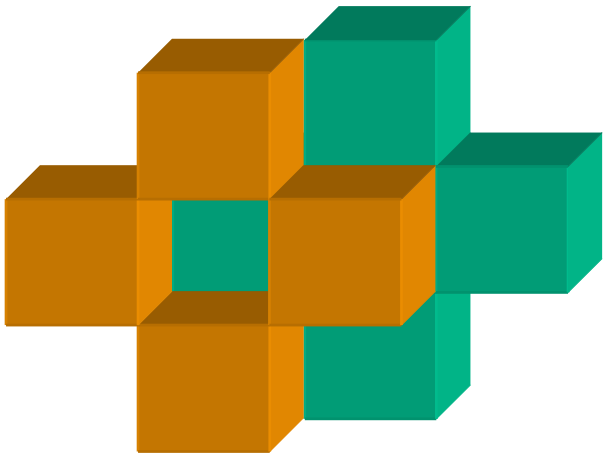
H. G. Scott,
Phase relationships in the zirconia-yttria system
JOURNAL OF MATERIALS SCIENCE 10 (1975) 1527-1535

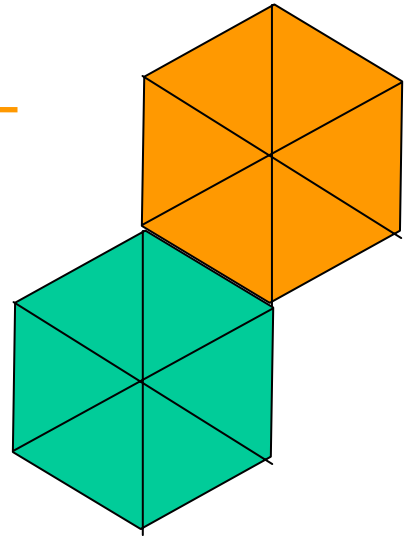


Fluorite oxides are highly radiation tolerant because they are able to accomodate point defects easily: *Science* **289** (2000) 748.

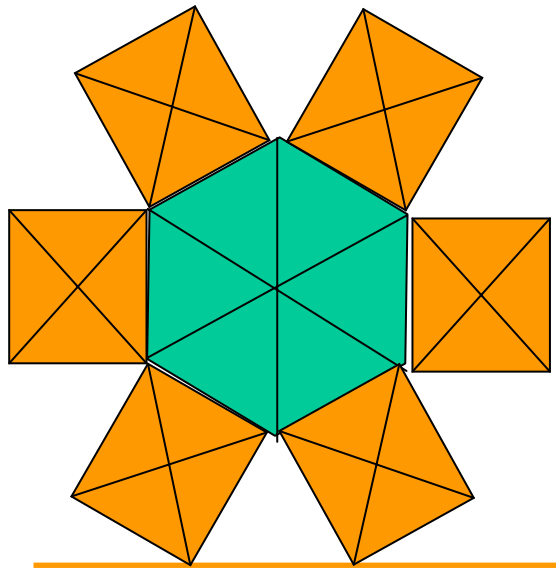
Class 7: Fluorite, pyrochlore, murataite

Fluorite





8 coordination + 8 coordination

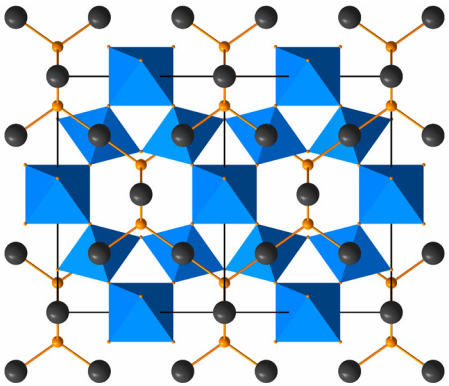


Pyrochlore

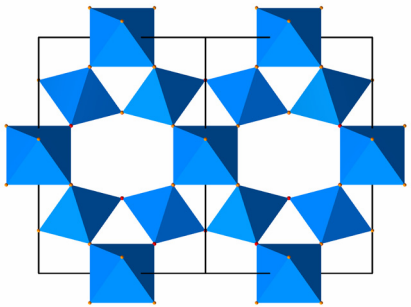
$A_2B_2O_8 \rightarrow A_2B_2O_7$

8 coordination + 6 coordination

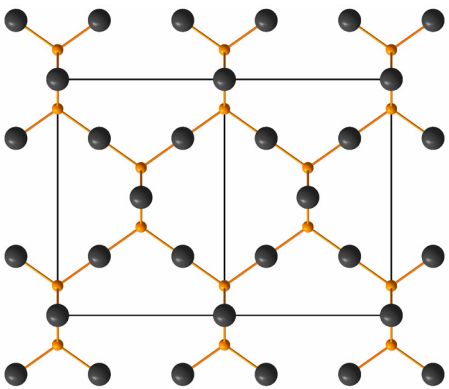
Pyrochlore views:



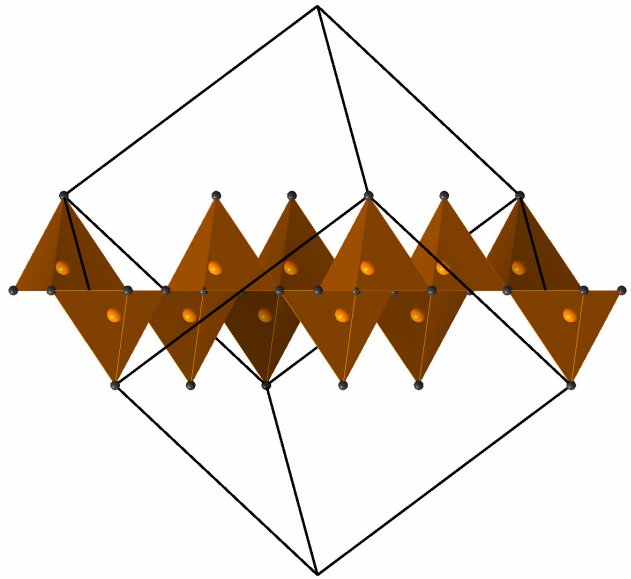
$A_2B_2O_6O'$



B_2O_6



A_2O'



Stellated *Kagomé* lattice of B_4 tetrahedra. The central atom is O′. This is a motif found in spinel as well.

Class 7: Fluorite, pyrochlore, murataite

A wide variety of pyrochlore structures are known: A can be Ca, Cd, Tl, Pb, Bi, Ln etc. B can be transition metals as well as main group elements. The A and B sites can be mixed. O′ can be absent, or can be F^-, OH^- etc.

Pyrochlores can be insulating, metallic, magnetic ...

The standard reference: Subramanian *et al*. Prog. Solid State Chem. **15** (1983) 55.

For unusual phase relationships in pyrochlores, see Vanderah *et al*. Eur. J. Inorg. Chem. (2005) 2895.

Murataites:

Urusov et al. Dokl. Earth Sci. 401 (2005) 315: Synthetic “murataites” as modular members of a pyrochlore-murataite polysomatic series.

The fluorite is a 3D chessboard of regular cubes. The pyrochlore has one half of the cubes replaced by octahedra, and one eights of the anions missing. The pyrochlore can be constructed by making the coloring the fluorite chessboard. This is a 2x2x2 ordering.

More complex 3x3x3 ordering gives the murataite.