Class 3: The crystal structures of High-T_c copper oxides

References:

- R. J. Cava, Oxide Superconductors, *J. Am. Ceram. Soc.* **83** (2000) 5-28.
- J. Orenstein and A. J. Millis, Advances in the physics of high-temperature superconductivity, Science 288 (2000) 468-474. Link to DOI
- E. Pavarini *et al*. Band-structure trend in hole-doped cuprates and correlation with $T_{c\ max}$, Phys. Rev. Lett. 87 (2001) 047003(1-4). Link to DOI

See also the second PDF file (addendum) for this class on general features of superconductors, and on R-P phases.

All high-T_c copper oxides can be described as possessing CuO_2 square planes and a charge reservoir that often comprises rock-salt like units.

In this class, we will examine the how perovskites can be thought to comprise rock-salt slabs interleaved with “perovskite” MO_2.

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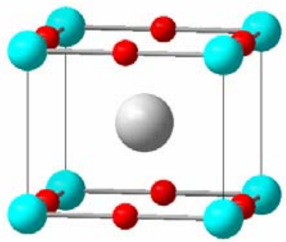

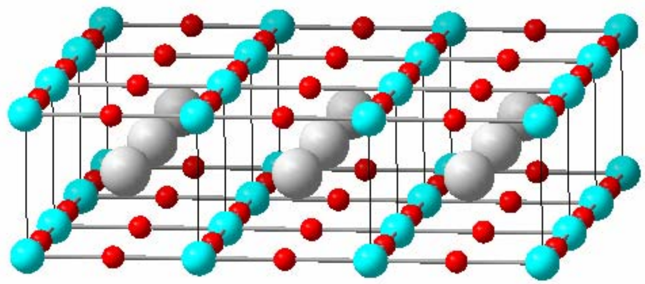

Views of the "parent" compound that only has CuO_2 sheets: $(Ca_{0.86}Sr_{0.14})CuO_2$

P4/mmm, a = 3.8611 Å, c = 3.1995 Å
Cu at 0 0 0
Ca/Sr at 0.5 0.5 0.5
O at 0 0.5 0

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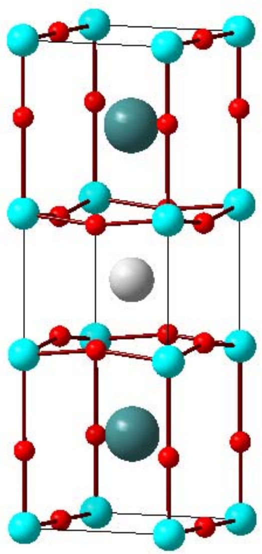
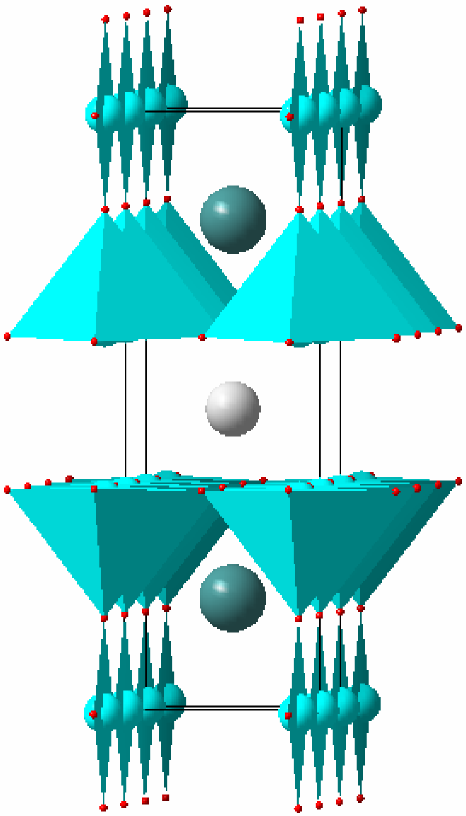


$YBa_2Cu_3O_7$ --- the "123" compound
Pmmm, a = 3.8203 Å, b = 3.8855 Å,
c = 11.6835 Å
Y at 0.5 0.5 0.5, Ba at 0.5 0.5 0.18393
Cu1 at 0 0 0, Cu2 at 0 0 0.3550
O1 at 0 0.5 0, O2 at 0.5 0 0.37819
O3 at 0 0.5 0.37693, O4 at 0 0 0.15840



Note the chains and sheets !

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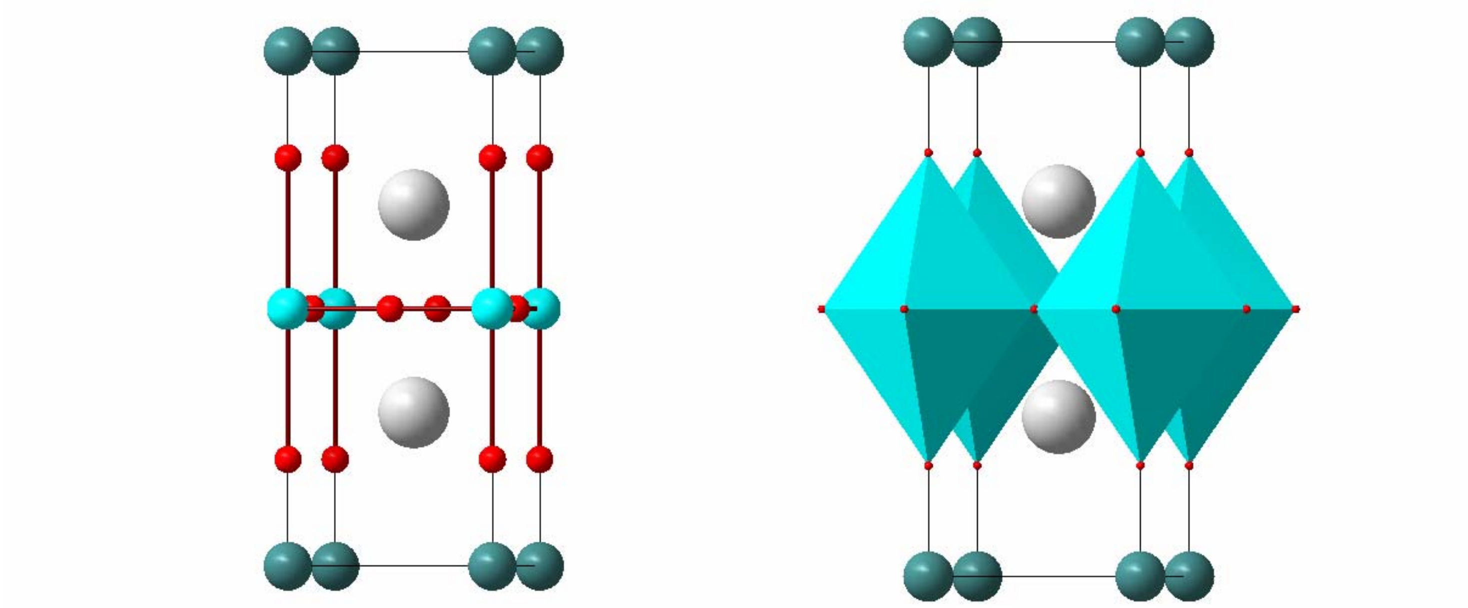

Note J-T distorted CuO_6 octahedra, and HgO_2 rods (linear)

$HgBa_2CuO_4$ --- the class of compounds with the highest T_c's.
P4/mmm, a = 3.87630 Å, c = 9.50720 Å
Hg at 0 0 0, Ba at 0.5 0.5 0.2986, Cu at 0 0 0.5,
O1 at 0.5 0 0.5 and O2 at 0 0 0.2075

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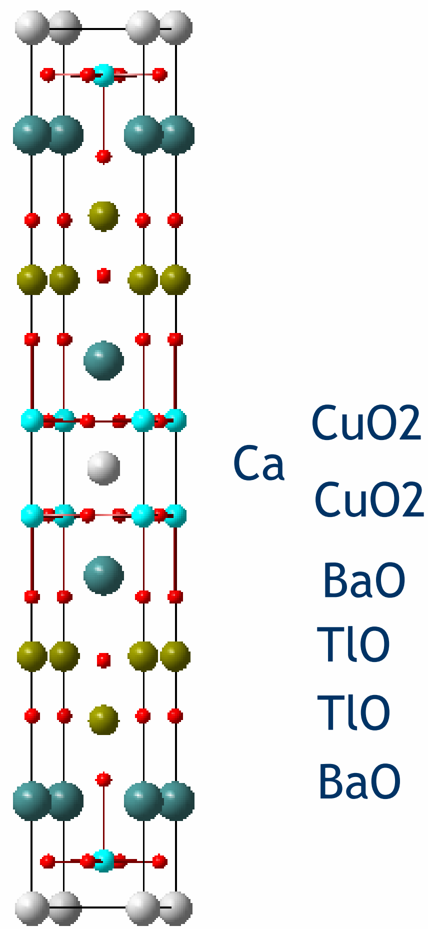

The O in the Tl layer is disordered.
This is not shown in this depiction.

The two-layer Tl-based superconductor, $Tl_2Ba_2CaCu_2O_8$
I4/mmm, a = 3.8550 Å, c = 29.318 Å

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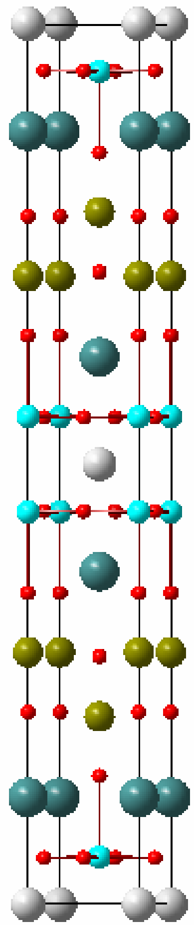

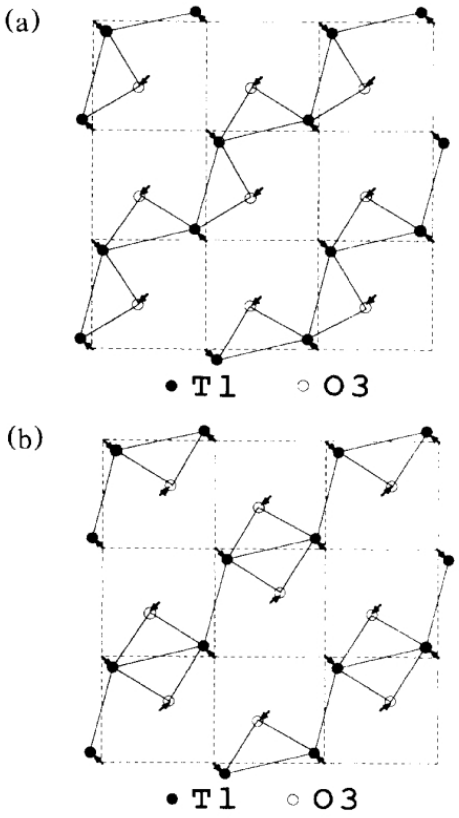

FIG. 2. The displacements of Tl and O3 atoms from the high-symmetry sites in the Tl-O3 plane for two idealized configurations. The ordering, however, is only short range, and the real stucture is most likely the random mixture of these two configurations (see text).

Dmowski *et al*. *Phys*. *Rev*. *Lett*. **61** (1988) 2608: PDF study of Tl and O local ordering.

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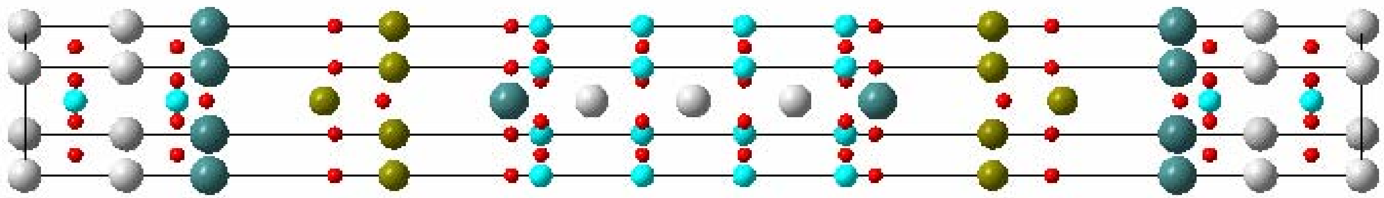

The 4-copper layer compound $Bi_2Sr_2Ca_3Cu_4O_{12}$

Many Bi superconductors display incommensurate modulation in the Bi-O layers. See for example, Petriček *et al*. *Phys*. *Rev*. *B* **42** (1990) 387.