Crystal chemistry of common mineral components

The valence state of Fe in the Fe-bearing components can easily be inferred from the charge balance. The abbreviation **T** in the structural formulas below denotes a tetrahedral (4-coordinated) position.

Upper mantle

Feldspars

Structural formula: **AT_4O_8**, where **A** is a large irregular position interstitial to the **T**O_4-tetrahedra

Plagioclase: anorthite, Ca $Al_2Si_2O_8$ albite, Na $AlSi_3O_8$

Alkali feldspar: orthoclase/K-feldspar, K $AlSi_3O_8$ albite, Na $AlSi_3O_8$

Silica minerals

Structural formula: **TO_2**, i.e. SiO_2

Pyroxenes

Structural formula: **M2 M1 T_2O_6**, where **M1** is a regular octahedral position. The **M2** position is an irregular position, which is 6-coordinated for the small Mg and Fe cations and 8-coordinated for the larger Ca and Na cations.

Orthopyroxene, opx: mainly enstatite, $Mg_2Si_2O_6$ ferrosilite, $Fe_2Si_2O_6$

Clinopyroxene, cpx: mainly diopside, $CaMgSi_2O_6$ hedenbergite, $CaFeSi_2O_6$
but also other components like:
- jadeite, $NaAlSi_2O_6$ in high-p pyroxenes and ægirine
- acmite, $NaFeSi_2O_6$ in clinopyroxenes in peralkaline rocks
- Ca-tschermak's component, CaAl AlSi O_6

Olivine

Structural formula: **M2 M1 TO_4**, where **M1** and **M2** are octahedral positions

Forsterite, Mg_2SiO_4 fayalite, Fe_2SiO_4

Garnet

Structural formula: **$A_3B_2T_3O_4$**, where **A** is an 8-coordinated position with divalent cations and **B** is a 6-coordinated position with trivalent cations (except in the majorite component which have 1 divalent cation + 1 Si^{4+} in **B**). In all of the garnet components, Si is the only tetrahedral cation.

Pyralspite garnets: pyrope, $Mg_3Al_2Si_3O_{12}$ almandine, $Fe_3Al_2Si_3O_{12}$ spessartine, $Mn_3Al_2Si_3O_{12}$

Ca-garnets: grossular, $Ca_3Al_2Si_3O_{12}$ andradite, $Ca_3Fe_2Si_3O_{12}$ uvarovite, $Ca_3Cr_2Si_3O_{12}$

An allocation of the ferric Fe into a component termed skiagite ($Fe_3Fe_2Si_3O_{12}$) is commonly used in oxygen barometry.

Majorite: Mg_3 MgSi Si_3O_{12}. One can also consider an Fe-equivalent majorite component: $Fe^{2+}{}_3$ $Fe^{2+}Si$ Si_3O_{12}

Spinel group

Spinel, $MgAl_2O_4$ magnetite, $Fe^{2+}Fe^{3+}{}_2O_4$ chromite, $FeCr_2O_4$

Carbonates

Calcite, $CaCO_3$ dolomite, $CaMg(CO_3)_2$ magnesite, $MgCO_3$

Transition zone and lower mantle

Wadsleyite and ringwoodite High-p olivine polymorphs, spinelloid- and spinel-structured, respectively. Wds: orthorombic, Rwd: isometric (cubic). **A_2TO_4**, where **A** includes three octahedral positions (M1, M2, M3).

Garnet. See composition and structure above. In the TZ and LM the majorite component makes up about or more than 50 mol%.

Ca-perovskite. **ABO_3**-compound close to $CaSiO_3$-composition. Near the solidus, cpv has the ideal isometric perovskite structure. At lower T, the symmetry is reduced to tetragonal.

Bridgmanite and post-bridgmanite. **ABO_3**-compounds, orthorombic symmetries. Dominant component: $MgSiO_3$. Other essential components are $MgAlO_{2.5}$ (limited to pressures less than about 40 GPa), $FeAlO_3$ (ferric Fe), $FeSiO_3$ (ferrous Fe) and Al_2O_3.

Silica minerals (in basaltic compositions). With increasing pressure, quartz, coesite, strishovite, b-stishovite, seifertite and pyrite-structured silica.

The Ca-ferrite-structured Al-rich phase (in basaltic compositions, CF-phase). Close to the compositional join between the components $(Mg,Fe)Al_2O_4$ and $NaAlSiO_4$. Orthorombic symmetry. Below 50 GPa there might also be a hexagonal version, referred to as the "new aluminous phase" or just NAL.