AX Mineral end-member activity models

Activities of mineral endmembers for thermobarometry may be calculated with the help of the program AX which accepts raw microprobe data in the form of oxide weight percents and performs standard mineral recalculations, with attempts at ferric iron estimation. The program calculates activities for end-members which can then be used for rock calculations in THERMOCALC . The assumptions used in deriving the activities and in estimation of ferric iron are listed briefly below. (R_{max} is the maximum allowed ratio of ferric to ferrous iron; ox is the number of oxygens, and cats is the number of cations in the formula unit; HP90 is Holland & Powell 1990, *J. Met. Geol.* **8**, 89–124. HP98 is Holland & Powell 1998, *J. Met. Geol.***16**, 309–343.)

See 1) HP90 p 100 & especially HP98 p 315–318
2) www pages at www.esc.cam.ac.uk/astaff/holland/

Mineral	**Ferric scheme**	**Notes on activity**
garnet	12 ox, 8 cats.	Regular soln. W's: py.alm=2.5, gr.py=41.4-0.0188T, py.andr=73, alm.andr=60, spss.andr=60kJ.
cpx, opx	6 ox, 4 cats.	2-sitemixing (Wood-Banno) with regular soln (opx: en-fs-mgts-di). cpx(di-hed-en-cats-jd-acm).
olivine	4 ox, 3 cats	2-site mixing W(MgFe)=4kJ
omphacite	6 ox, 4 cats.	Omph: ideal mixing 1-site model
ilmenite-hematite	3 ox, 2 cats.	2-site ideal mixing
talc	11 ox, 7 cats. R_{max} =0.10	Ideal site mixing - (HP90, p100)
cordierite	18 ox, 11 cats	2 site mixing+ nonideal (WFeMg=1.5 kJ, WMnMg=1.5 kJ)
chloritoid	6 ox, 4 cats. R_{max} =0.20	2 site mixing+ nonideal (WFeMg=1.5 kJ, WMnMg=1.5 kJ)
staurolite	All ferrous	4-site Fe-Mg ideal mixing
chlorite	14 ox, 10 cats. R_{max} =0.30	Holland, Baker & Powell (E.J.Min. **10**, 395–406)
biotite	11 ox, M1+M2+M3+T=6.9 R_{max} =0.15	see www page + non-ideal A-site mixing from (Eugster et al 1972, *J. Pet.* **13**, 147-179)
phengite, paragonite, margarite	11 ox, M1+M2+M3+T=6.05 R_{max} =0.50	Non-ideal mixing - see www pages

spinels	4 ox, 3 cats	Normal spinels: 2-site mixing, Whs=1.5, Whm=39, Wms=41 (kJ) [h=herc, m=mt, s=sp]. Inverse spinels - ideal mixing
sapphirine	20 ox, 14 cats	ideal mixing-on-sites: 2(Mg,Al)oct + 2(Al,Si)tet
osumilite	30 ox, 18 cats	ideal mixing-on-sites: [K,Na] (Mg,Fe)2 [Al,Mg,Fe]3 Si10 [Al,Si]2 O30
scapolite	16 cations	ideal-Al/Si ordered model
epidote	12.5 ox, $Si+Al+Fe^{3+} = 6.0$	2-site ordering model (HP98, see www pages)
carbonates	All ferrous	calcite, siderite: 1-site mixing; dolomite, ankerite: 2-site mixing (HP98)
alkali feldspar	All ferric	Waldbaum & Thompson 1969, subregular model
plagioclase	All ferric	Holland & Powell (1992) *Am Min*, **77**, 53-61. (model 1)
amphibole	Holland & Blundy (1993) *Cont. Min. Pet.* **116**, 433-447	Mixing model: Dale, Holland & Powell (CMP in review)