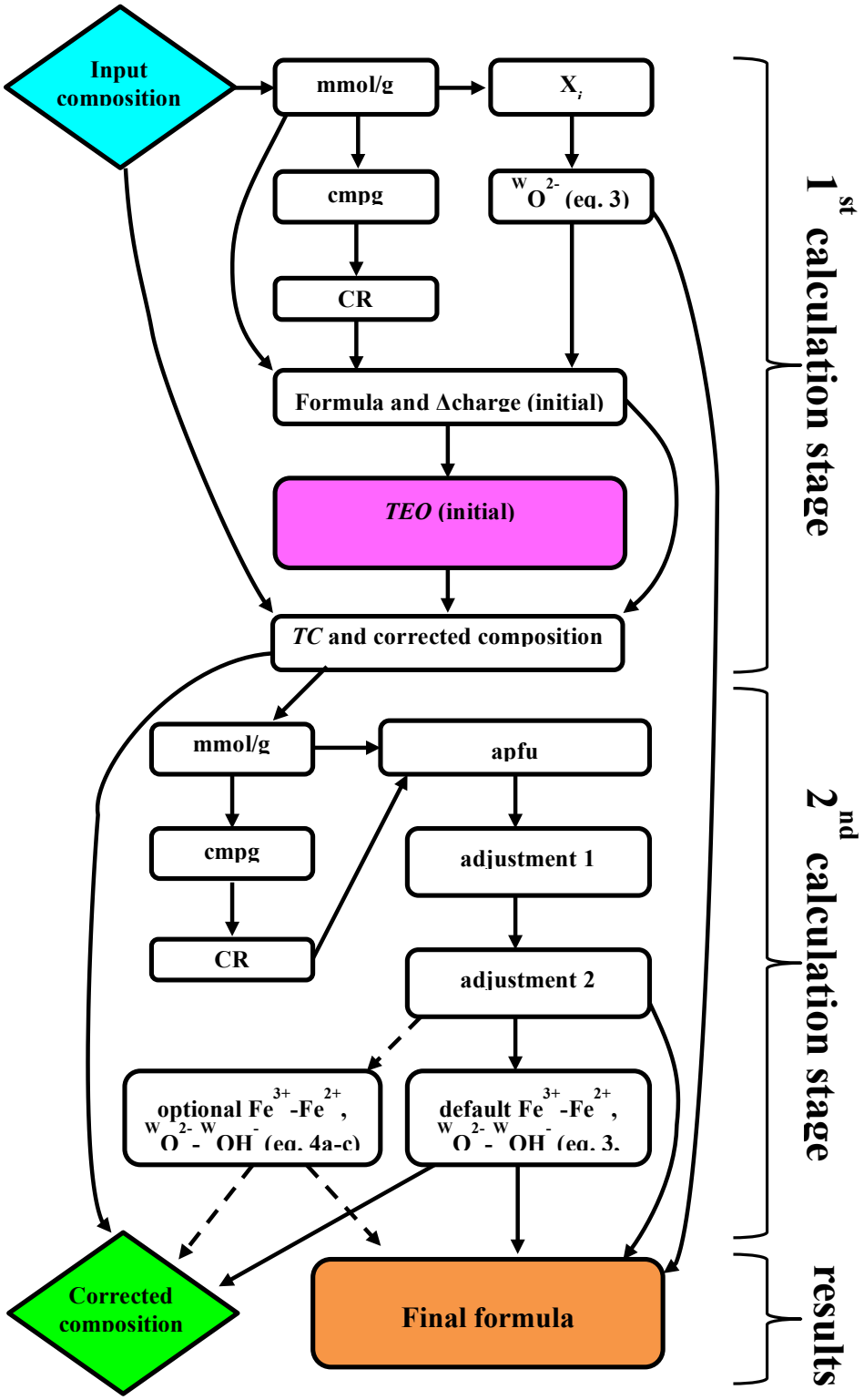
# APPENDIX 1

## Flow–chart and Commands in Excel to build an AMFORM model

(colors highlight the input and results of the AMFORM.xlsx spreadsheet; hidden and data calculations are not colored)



***Operative definitions***

$A_r^i$: atomic mass of *i* (u);

$M_r^i$: molecular mass of *i* (g/mol);

$X_i$: mass of *i* divided by the total cation mass;

$^{T}i$: element *i* in the T group-sites;

$^{C}i$: element *i* in the C group-sites;

$^{C\pm B}i$: element *i* in the C and/or B group-sites;

$^{B\pm A}i$: element *i* in the B and/or A group-sites;

$^{B}i$: element *i* in the B group-sites;

$^{A}i$: element *i* in the A group-sites;

$^{W}i$: element *i* in the W group-sites;

ΔC: amount of Mg + $Fe^{2+}$ + Mn in the B group-sites;

Δcharge: positive – negative charges (deviation from electroneutrality);

[*n*].: calculation *n* (ex. [*n*]. = identifier = values or calculation);

[*n*]: resulting value of calculation in [*n*];

"…": unit of measurement.

***Input composition (original)***

$SiO_2$ = input "wt%"

$TiO_2$ = input "wt%"

$Al_2O_3$ = input "wt%"

$Cr_2O_3$ = input "wt%"

$FeO_{tot}$ = input "wt%" (iron expressed as FeO)

MnO = input "wt%"

(NiO + ZnO) = input "wt%"

MgO = input "wt%"

CaO = input "wt%"

$Na_2O$ = input "wt%"

$K_2O$ = input "wt%"

F = input "wt%"

Cl = input "wt%"

***1st calculation stage***

<u>mmol/g, cmpg (cation mass per gram) and CR (correlation ratio) calculations from the original composition:</u>

[1]. Si "mmol/g" = $SiO_2*10/M_r^{SiO2}$
[2]. Ti "mmol/g"= $TiO_2*10/M_r^{TiO2}$
[3]. Al "mmol/g"= $Al_2O_3*20/M_r^{Al2O3}$
[4]. Cr "mmol/g" = $Cr_2O_3*20/M_r^{Cr2O3}$
[5]. Fe "mmol/g" = $FeO_{tot}*10/M_r^{FeO}$
[6]. Mn "mmol/g" = $MnO*10/M_r^{MnO}$
[7]. Ni+Zn "mmol/g" = $(NiO + ZnO)*10/M_r^{NiO}$
[8]. Mg "mmol/g"= $MgO*10/M_r^{MgO}$
[9]. Ca "mmol/g" = $CaO*10/M_r^{CaO}$
[10]. Na "mmol/g" = $Na_2O*20/M_r^{Na2O}$
[11]. K "mmol/g" = $K_2O*20/M_r^{K2O}$
[12]. ∑Si→K "mmol/g"= SUM([1]:[11])
[13]. F "mmol/g" = $F*10/A_r^F$
[14]. Cl "mmol/g" = $Cl*10/A_r^{Cl}$
[15]. cmpg = $10^{-2}$∑Si→K "wt%" = ([1]*$A_r^{Si}$ + [2]*$A_r^{Ti}$ + [3]*$A_r^{Al}$ + [4]*$A_r^{Cr}$ + [5]*$A_r^{Fe}$ + [6]*$A_r^{Mn}$ + [7]*$A_r^{Ni}$ + [8]*$A_r^{Mg}$ + [9]*$A_r^{Ca}$ + [10]*$A_r^{Na}$ + [11]*$A_r^{K}$)/1000
[16]. CR = $4.809*[15]^2 - 3.409*[15] + 1.276$

<u>$X_i$ and $^{W}O^{2-}$ calculations:</u>

[17]. $X_{Si}$ = [1]*$A_r^{Si}*10^{-3}$/[15]
[18]. $X_{Ti}$ = [2]*$A_r^{Ti}*10^{-3}$/[15]
[19]. $X_{Al}$ = [3]*$A_r^{Al}*10^{-3}$/[15]
[20]. $X_{Fe}$ = [5]*$A_r^{Fe}*10^{-3}$/[15]
[21]. $X_{Mn}$ = [6]*$A_r^{Mn}*10^{-3}$/[15]
[22]. $X_{Mg}$ = [8]*$A_r^{Mg}*10^{-3}$/[15]
[23]. $X_{Ca}$ = [I9]*$A_r^{Ca}*10^{-3}$/[15]
[24]. $X_{Na}$ = [10]*$A_r^{Na}*10^{-3}$/[15]
[25]. $X_K$ = [11]*$A_r^{K}*10^{-3}$/[15]
[26]. $X_F$ = [13]*$A_r^{F}*10^{-3}$/[15]
[27]. $^{W}O^{2-}$ "apfu" calculated = $-6.684*[17] + 11.025*[18] - 0.989*[19] - 2.800*[20] - 20.359*[21] - 0.903*[22] - 6.875*[23] - 11.119*[24] - 2.553*[25] + 5.751*[26] + 4.610$
[28]. $^{W}O^{2-}$ "apfu" adjustement1 = IF([27] < 0; 0; [27])

<u>apfu and *TEO* calculations from the original composition:</u>

[29]. Si "apfu" = [1]*[16]
[30]. Ti "apfu" = [2]*[16]
[31]. Al "apfu" = [3]*[16]
[32]. Cr "apfu" = [4]*[16]
[33]. Fe "apfu" = [5]*[16]
[34]. Mn "apfu" = [6]*[16]
[35]. Ni+Zn "apfu" = [7]*[16]
[36]. Mg "apfu" = [8]*[16]
[37]. Ca "apfu" = [9]*[16]
[38]. Na "apfu" = [10]*[16]
[39]. K "apfu" = [11]*[16]
[40]. ∑Si→K "apfu" = [12]*[16]
[41]. F "apfu" = [13]*[16]
[42]. Cl "apfu" = [14]*[16]
[43]. charge – "apfu" = 46 + [28]
[44]. minimum charge + "apfu" = [29]*4 + [30]*4 + [31]*3 + [32]*3 + [33]*2 + [34]*2 + [35]*2 + [36]*2 + [37]*2 + [38] + [39]
[45]. $Fe^{3+}$ "apfu" = IF([43] – [44] < 0; 0; IF([43] – [44] > [33]; [33]; [43] – [44]))

[46]. $Fe^{2+}$ "apfu" = [33] – [45]
[47]. $^{T}$Si "apfu" = [29]
[48]. $^{T}$Al "apfu" = IF(8 – [47] < [31]; 8 – [47]; [31])
[49]. $^{T}$Ti "apfu" = IF(8 – [47] – [48] > 0; 8 – [47] – [48]; 0)
[50]. $^{C}$Al "apfu" = [31] – [48]
[51]. $^{C}$Ti "apfu" = [30] – [49]
[52]. $^{C}$Cr "apfu" = [32]
[53]. $^{C}$Ni+Zn "apfu" = [35]
[54]. $^{C}Fe^{3+}$ "apfu" = [45]
[55]. $^{C\pm B}$Mg "apfu" = [36]
[56]. $^{C\pm B}Fe^{2+}$ "apfu" = [46]
[57]. $^{C\pm B}$Mn "apfu" = [34]
[58]. ΔC "apfu" = SUM([47]:[57]) – 13
[59]. $^{B\pm A}$Ca "apfu" = [37]
[60]. $^{B}$Na "apfu" = IF([58] + [59] > 2; 0; 2 – [58] – [59])
[61]. $^{B}$Ca "apfu" = [58] + [59] + [60] – 2
[62]. $^{A}$Na "apfu" = [38] – [60]
[63]. $^{A}$K "apfu" = [39]
[64]. $^{A}$(Ca+Na+K) "apfu" = [61] + [62] + [63]
[65]. $^{W}$F "apfu" = [41]
[66]. $^{W}$Cl "apfu" = [42]
[67]. $^{W}$O "apfu" = [28]
[68]. $^{W}$OH "apfu" = 2 – [65] – [66] – [67]
[69]. Δcharge "apfu" = ([47] + [49] + [51])*4 + ([48] + [50] + [52] + [54]}*3 + ([53] + [55] + [56] + [57] + [59])*2 + [60] + [62] + [63] – ([65] + [66] + [68]) – (22 + [67])*2
[70]. $Fe^{3+}/(Fe^{3+} + Fe^{2+})$ = [45]/([45] + [46])
[71]. $Fe_2O_3$ "wt%" = [70]*[5]*$M_r^{Fe2O3}$/20
[72]. FeO "wt%" = [5]*$M_r^{FeO}$/[70]/10
[73]. O=F,Cl "wt%" = –(F "wt%"/$A_r^{F}$ + Cl "wt%"/$A_r^{Cl}$)*$A_r^{O}$/2;
[74]. $H_2O$ "wt%" = [68]*$M_r^{H2O}$/[16]/20
[75]. *TEO* "wt%" = $SiO_2$ "wt%" + $TiO_2$ "wt%" + $Al_2O_3$ "wt%" + $Cr_2O_3$ "wt%" + MnO "wt%" + (NiO + ZnO) "wt%" + MgO "wt%" + CaO "wt%" + $Na_2O$ "wt%" + $K_2O$ "wt%" + F "wt%" + Cl "wt%" + SUM([71]:[74])

Calculation of the corrected composition

[76]. $$TC = -7.942 * 10^{-4} * SiO_2{}^{wt\%} + 6.000 * 10^{-4} * TiO_2{}^{wt\%} - 6.566 * 10^{-4} * Al_2O_3{}^{wt\%} + 8.754 * 10^{-5} * [71] - 9.391 * 10^{-4} * [72] - 8.501 * 10^{-4} * MgO^{wt\%} - 1.104 * 10^{-3} * CaO"wt\%" - 1.477 * 10^{-3} * Na_2O"wt\%" - 8.608 * 10^{-4} * K_2O"wt\%" - 9.619 * 10^{-3} * [73] + 6.414 * 10^{-3} * [74] - 9.568 * 10^{-3} * [75] + 4.130 * 10^{-4} * [69] + 2.024$$
[77]. $SiO_2$ "wt%" corrected = $SiO_2$ "wt%"*[76]
[78]. $TiO_2$ "wt%" corrected = $TiO_2$ "wt%"*[76]
[79]. $Al_2O_3$ "wt%" corrected = $Al_2O_3$ "wt%"*[76]
[80]. $Cr_2O_3$ "wt%" corrected = $Cr_2O_3$ "wt%"*[76]
[81]. $FeO_{tot}$ "wt%" corrected = $FeO_{tot}$ "wt%"*[76]
[82]. MnO "wt%" corrected = MnO "wt%"*[76]
[83]. (NiO + ZnO) "wt%" corrected = (NiO + ZnO) "wt%"*[76]
[84]. MgO "wt%" corrected = MgO "wt%"*[76]
[85]. CaO "wt%" corrected = CaO "wt%"*[76]
[86]. $Na_2O$ "wt%" corrected = $Na_2O$ "wt%"*[76]
[87]. $K_2O$ "wt%" corrected = $K_2O$ "wt%"*[76]
[88]. F "wt%" corrected = F "wt%"*[76]
[89]. Cl "wt%" corrected = Cl "wt%"*[76]

***2nd calculation stage***

mmol/g, cmpg (cation mass per gram) and CR (correlation ratio) calculations from the corrected composition:

[90]. Si "mmol/g" = [77]*10/$M_r^{SiO2}$
[91]. Ti "mmol/g" = [78]*10/$M_r^{TiO2}$
[92]. Al "mmol/g" = [79]*20/$M_r^{Al2O3}$
[93]. Cr "mmol/g" = [80]*20/$M_r^{Cr2O3}$
[94]. Fe "mmol/g" = [81]*10/$M_r^{FeO}$
[95]. Mn "mmol/g" = [82]*10/$M_r^{MnO}$
[96]. Ni+Zn "mmol/g" = [83]*10/$M_r^{NiO}$
[97]. Mg "mmol/g" = [84]*10/$M_r^{MgO}$
[98]. Ca "mmol/g" = [85]*10/$M_r^{CaO}$
[99]. Na "mmol/g" = [86]*20/$M_r^{Na2O}$
[100]. K "mmol/g" = [87]*20/$M_r^{K2O}$
[101]. ∑Si→K "mmol/g" = SUM([90]:[100])
[102]. F "mmol/g" = [88]*10/$A_r^{F}$
[103]. Cl "mmol/g" = [89]*10/$A_r^{Cl}$
[104]. cmpg = $10^{-2}$∑Si→K "wt%" = ([90]*$A_r^{Si}$ + [91]*$A_r^{Ti}$ + [92]*$A_r^{Al}$ + [93]*$A_r^{Cr}$ + [94]*$A_r^{Fe}$ + [95]*$A_r^{Mn}$ + [96]*$A_r^{Ni}$ + [97]*$A_r^{Mg}$ + [98]*$A_r^{Ca}$ + [99]*$A_r^{Na}$ + [100]*$A_r^{K}$)/1000
[105]. CR = 4.809*[104]$^2$ – 3.409**[104] + 1.276

Formula calculations from the corrected composition:

[106]. Si "apfu" = [90]*[105]
[107]. Ti "apfu" = [91]*[105]
[108]. Al "apfu" = [92]*[105]
[109]. Cr "apfu" = [93]*[105]
[110]. Fe "apfu" = [94]*[105]
[111]. Mn "apfu" = [95]*[105]
[112]. Ni+Zn "apfu" = [96]*[105]
[113]. Mg "apfu" = [97]*[105]
[114]. Ca "apfu" = [98]*[105]
[115]. Na "apfu" = [99]*[105]
[116]. K "apfu" = [100]*[105]
[117]. F "apfu" = [102]*[105]
[118]. Cl "apfu" = [103]*[105]
[119]. ∑Si→K "apfu" = SUM([106]:[116])
[120]. ∑Si→Mg "apfu" = SUM([106]:[113])
[121]. ∑Si→Al "apfu" = SUM([106]:[108])
[122]. Si "apfu" adjustment1 = IF([120] < 13; [106]*13/[120]; IF([119] > 16; [106]*16/[119]; [106]))
[123]. Ti "apfu" adjustment1 = IF([120] < 13; [107]*13/[120]; IF([119] > 16; [107]*16/[119]; [107]))
[124]. Al "apfu" adjustment1 = IF([120] < 13; [108]*13/[120]; IF([119] > 16; [108]*16/[119]; [108]))
[125]. Cr "apfu" adjustment1 = IF([120] < 13; [109]*13/[120]; IF([119] > 16; [109]*16/[119]; [109]))
[126]. Fe "apfu" adjustment1 = IF([120] < 13; [110]*13/[120]; IF([119] > 16; [110]*16/[119]; [110]))
[127]. Mn "apfu" adjustment1 = IF([120] < 13; [111]*13/[120]; IF([119] > 16; [111]*16/[119]; [111]))
[128]. Ni+Zn "apfu" adjustment1 = IF([120] < 13; [112]*13/[120]; IF([119] > 16; [112]*16/[119]; [112]))
[129]. Mg "apfu" adjustment1 = IF([120] < 13; [113]*13/[120]; IF([119] > 16; [113]*16/[119]; [113]))
[130]. Ca "apfu" adjustment1 = IF([120] < 13; [114]*13/[120]; IF([119] > 16; [114]*16/[119]; [114]))
[131]. Na "apfu" adjustment1 = IF([120] < 13; [115]*13/[120]; IF([119] > 16; [115]*16/[119]; [115]))

[132]. K "apfu" adjustment1 = IF([120] < 13; [116]*13/[120]; IF([119] > 16; [116]*16/[119]; [116]))
[133]. F "apfu" adjustment1 = IF([120] < 13; [117]*13/[120]; IF([119] > 16; [117]*16/[119]; [117]))
[134]. Cl "apfu" adjustment1 = IF([120] < 13; [118]*13/[120]; IF([119] > 16; [118]*16/[119]; [118]))
[135]. ∑Si→K "apfu" = SUM([122]:[132])
[136]. ∑Si→Mg "apfu" = SUM([122]:[129])
[137]. ∑Si→Al = SUM([122]:[124])
[138]. Si "apfu" adjustment2 = IF([122] > 8; 8; IF([137] < 8; [122]*8/[137]; IF([135] > 16; [122]*16/[135]; [122])))
[139]. Ti "apfu" adjustment2 = IF([122] > 8; [123]*8/[122]; IF([137] < 8; [123]*8/[137]; IF([135] > 16; [123]*16/[135]; [123])))
[140]. Al "apfu" adjustment2 = IF([122] > 8; [124]*8/[122]; IF([137] < 8; [124]*8/[137]; IF([135] > 16; [124]*16/[135]; [124])))
[141]. Cr "apfu" adjustment2 = IF([122] > 8; [125]*8/[122]; IF([137] < 8; [125]*8/[137]; IF([135] > 16; [125]*16/[135]; [125])))
[142]. Fe "apfu" adjustment2 = IF([122] > 8; [126]*8/[122]; IF([137] < 8; [126]*8/[137]; IF([135] > 16; [126]*16/[135]; [126])))
[143]. Mn "apfu" adjustment2 = IF([122] > 8; [127]*8/[122]; IF([137] < 8; [127]*8/[137]; IF([135] > 16; [127]*16/[135]; IF([135] < 15; [127]*15/[135]; [127])))
[144]. Ni+Zn "apfu" adjustment2 = IF([122] > 8; [128]*8/[122]; IF([137] < 8; [128]*8/[137]; IF([135] > 16; [128]*16/[135]; IF([135] <15; [128]*15/[135]; [128])))
[145]. Mg "apfu" adjustment2 = IF([122] > 8; [129]*8/[122]; IF([137] < 8; [129]*8/[137]; IF([135] > 16; [129]*16/[135]; IF([135] <15; [129]*15/[135]; [129])))
[146]. Ca "apfu" adjustment2 = IF([122] > 8; [130]*8/[122]; IF([137] < 8; [130]*8/[137]; IF([135] > 16; [130]*16/[135]; IF([135] <15; [130]*15/[135]; [130])))
[147]. Na "apfu" adjustment2 = IF([122] > 8; [131]*8/[122]; IF([137] < 8; [131]*8/[137]; IF([135] > 16; [131]*16/[135]; IF([135] <15; [131]*15/[135]; [131])))
[148]. K "apfu" adjustment2 = IF([122] > 8; [132]*8/[122]; IF([137] < 8; [132]*8/[137]; IF([135] > 16; [132]*16/[135]; IF([135] <15; [132]*15/[135]; [132])))
[149]. F "apfu" adjustment2 = IF([122] > 8; [133]*8/[122]; IF([137] < 8; [133]*8/[137]; IF([135] > 16; [133]*16/[135]; IF([135] <15; [133]*15/[135]; [133])))
[150]. Cl "apfu" adjustment2 = IF([122] > 8; [134]*8/[122]; IF([137] < 8; [134]*8/[137]; IF([135] > 16; [134]*16/[135]; IF([135] <15; [134]*15/[135]; [134])))
[151]. $^{T}$Si "apfu" = [138]
[152]. $^{T}$Al "apfu" = IF(8 – [151] < [140]; 8 – [151]; [140])
[153]. $^{T}$Ti "apfu" = IF(8 – [151] – [152] > 0; 8 – [151] – [152]; 0)
[154]. $^{C}$Al "apfu" = [140] – [152]
[155]. $^{C}$Ti "apfu" = [139] – [153]
[156]. charge – "apfu" adjustment1 = 46 + [28]
[157]. minimum charge + "apfu" = [138]*4 + [139]*4 + [140]*3 + [141]*3 + [142]*2 + [143]*2 + [144]*2 + [145]*2 + [146]*2 + [147] + [148]
[158]. $^{W}O^{2-}$ "apfu" adjustment2 = IF(2*[155] – [28] < 0, 2*[155]; IF([156] – [157] > 0; [28]; [157] – 46))
[159]. charge – "apfu" adjustment2 = 46 + [158];
[160]. $Fe^{3+}$ "apfu" = IF([156] – [157] < 0; 0; IF([159] – [157] > [142]; [142]; IF([159] – [157] < 0; 0; [159] – [157])))
[161]. $Fe^{2+}$ "apfu" = [142] – [160]
[162]. $Fe^{3+}/(Fe^{3+} + Fe^{2+})$ = [160]/([160] + [161])
[163]. $^{W}OH^{-}$ "apfu" = 2 – [149] – [150] – [158]

Optional $Fe^{3+}$, $^{W}O^{2-}$ and $^{W}OH^{-}$ calculations:

[164]. $^{B}$Na "apfu" = IF(SUM([138]:[145]) – 13 + [146] > 2; 0; IF(2 – (SUM([138]:[145]) – 13) – [146] < [147]; 2 – (SUM([138]:[145]) – 13) – [146]; [147]))
[165]. $^{A}$Na "apfu" = IF(SUM([138]:[146]) > 15; [147]; [147] – 15 + SUM([138]:[146]))
[166]. $^{W}$O "apfu" = IF(3*(4/3*[155] + 2/3*(46 – 4*([151] + [153] + [155]) – 3*([152] + [154] + [141]) – 2*([144] + [145] + [143] + [160] + [161] + [146]) - [147] - [148]) + 2/3*( [165] + [148]) – 2/3) < 0; 0; IF(3*(4/3*[155] + 2/3*(46 – 4*([151] + [153] + [155]) – 3*([152] + [154] + [141]) – 2*([144] + [145] + [143] + [160] + [161] + [146]) - [147] - [148]) + 2/3*( [165] + [148]) – 2/3) > 2 - [149] - [150]; 2 - [149] - [150]; 3*(4/3*[155] + 2/3*(46 – 4*([151] + [153] + [155]) – 3*([152] + [154] + [141]) – 2*([144] + [145] + [143] + [160] + [161] + [146]) - [147] - [148]) + 2/3*([155] + [148]) – 2/3))
[167]. $^{C}Fe^{3+}$ "apfu" = 46 + [166] – 4*([151] + [153] + [155]) – 3*([152] + [154] + [141]) – 2*([144] + [145] + [143] + [160] + [161] + [146]) - [147] - [148]
[168]. $Fe^{3+}$ "apfu" adjustement3 = IF([167] < 0; 0; IF([167] > [142]; [142]; [167]))
[169]. $^{W}$O "apfu" adjustement3 = 4*([138] + [139]) + 3*([140] + [141]) + 2*(SUM([142] :[146]) +[147] + [148] + [168] – 46)
[170]. $Fe^{2+}$ "apfu" = [142] – [168]
[171]. $Fe^{3+}/(Fe^{3+} + Fe^{2+})$ = [168]/([168] + [170])
[172]. $^{W}OH^{-}$ "apfu" = 2 – [149] – [150] – [169]

***Output***

Corrected composition:
$SiO_2$ "wt%" = [77]
$TiO_2$ "wt%" = [78]
$Al_2O_3$ "wt%" = [79]
$Cr_2O_3$ "wt%" = [80]
$FeO_{tot}$ "wt%" = [81]
MnO "wt%" = [82]
(NiO + ZnO) "wt%" = [83]
MgO "wt%" = [84]
CaO "wt%" = [85]
$Na_2O$ "wt%" = [86]
$K_2O$ "wt%" = [87]
F "wt%" = [88]
Cl "wt%" = [89]
Sum "wt%" = SUM([77]:[89])
$Fe_2O_3$ "wt%" = [162]*[94]*$M_r^{Fe2O3}$/20 or [171]*[94]*$M_r^{Fe2O3}$/20
FeO "wt%" = [94]*$M_r^{FeO}$/[162]/10 or [94]*$M_r^{FeO}$/[171]/10
O=F,Cl "wt%" = – ([88]/$A_r^{F}$ + [89]/$A_r^{Cl}$)*$A_r^{O}$/2

$H_2O$ "wt%" = [163]*([90]/[151])*$M_r^{H2O}$/[105]/20 or
[172]*([90]/[151])*$M_r^{H2O}$/[105]/20
*TEO* "wt%" = SUM([77]:[80]) + SUM([82]:[89]) +
[162]*[94]*$M_r^{Fe2O3}$/20 + [94]*$M_r^{FeO}$/[162]/10 – ([88]/$A_r^{F}$ +
[89]/$A_r^{Cl}$)*$A_r^{O}$/2 + [163]*([90]/[151])*$M_r^{H2O}$/[105]/20

Final formula:
$^{T}$Si "apfu" = [151]
$^{T}$Al "apfu" = [152]
$^{T}$Ti "apfu" = [153]
$^{C}$Al "apfu" = [154]
$^{C}$Ti "apfu" = [155]
$^{C}$Cr "apfu" = [141]
$^{C}$Ni+Zn "apfu" = [144]
$^{C}Fe^{3+}$ "apfu" = [160] or [168]
$^{C+B}$Mg "apfu" = [145]
$^{C+B}Fe^{2+}$ "apfu" = [161] or [170]
$^{C+B}$Mn "apfu" = [143]
ΔC "apfu" = SUM([138]:[145]) – 13
$^{B}$Ca "apfu" = IF(ΔC "apfu" + [146] > 2; 2 – ΔC "apfu"; [146])
$^{B}$Na "apfu" = IF(ΔC "apfu" + $^{B}$Ca "apfu" > 2; 0; 2 - ΔC "apfu"
- $^{B}$Ca "apfu"))
$^{A}$Ca "apfu" = IF([146] > $^{B}$Ca "apfu"; [146] - $^{B}$Ca "apfu"; 0)
$^{A}$Na "apfu" = IF([147] > $^{B}$Na "apfu"; [147] – $^{B}$Na "apfu"; 0)
$^{A}$K "apfu" = [148]
$^{A}$(Ca+Na+K) = SUM([138]:[148]) – 15
$^{W}$F "apfu" = [149]
$^{W}$Cl "apfu" = [150]
$^{W}$OH "apfu" = [163] or [172]
$^{W}$O "apfu" = [158] or [169]