Adjustment of major elements used for computing the isometric log-ratio transformations.

When Fe2O3t concentration is not reported; i.e., when either FeOt or both Fe2O3 and FeO are available, the following simple equation is used for calculating Fe2O3 t from the reported data:

Function Equation for adjustment

Fe2O3t = Fe2O3 + [FeO × 159.6882/(2 × 71.8444) ]

SiO2A = 100 × SiO2/ [SiO2 + TiO2 + Al2O3+ Fe2O3t+ MnO + MgO + CaO + Na2O + K2O + P2O5)]

TiO2A = 100 × TiO2/ [SiO2 + TiO2 + Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)]

Al2O3A = 100 × Al2O3/ [SiO2 + TiO2 + Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)]

Fe2O3tA = 100 × Fe2O3t/ [SiO2 + TiO2 + Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)]

MnOA = 100 × MnO /[ SiO2 + TiO2+ Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)]

MgOA = 100 × MgO /[ SiO2 + TiO2 + Al2O3 + Fe2O3t+ MnO + MgO + CaO + Na2O + K2O + P2O5)]

CaOA = 100 × CaO/ [SiO2 + TiO2 + Al2O3 + Fe2O3t+ MnO + MgO + CaO + Na2O + K2O + P2O5)]

Na2OA = 100 × Na2O/ [SiO2 + TiO2 + Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)]

K2OA = 100 × K2O/ [SiO2 + TiO2 + Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)

P2O5A = 100 × P2O5 [SiO2 + TiO2 + Al2O3 + Fe2O3t + MnO + MgO + CaO + Na2O + K2O + P2O5)]

Isometric log-ratio transformation equations for major elements (the function ln represents natural

logarithm; the final letter A after chemical symbols refer to the adjusted concentrations on an anhydrous basis to

100% with total Fe as Fe2O3t).

Isometric Equation for transformation

log-ratios

ilr1TiM  = √ 1/2 × ln{ SiO2A / TiO2A }

ilr2AlM = √ 2/3 × ln{[2√( SiO2A × TiO2A) ]/ Al2O3A }

ilr3FeM = √ 3/4 × ln{[3√( SiO2A × TiO2A × Al2O3A)] / Fe2O3tA }

ilr4MnM  = √ 4/5 × ln{[4√( SiO2A × TiO2A × Al2O3A × Fe2O3tA) ]/MnOA}

ilr5MgM = √ 5/6 × ln{[5√( SiO2A × TiO2A × Al2O3A × Fe2O3tA × MnOA) ]/MgOA}

ilr6CaM = √ 6/7 × ln{[6√( SiO2A × TiO2A × Al2O3A × Fe2O3tA × MnOA × MgOA)]/CaOA}

ilr7NaM = √ 7/8 × ln{[7√( SiO2A × TiO2A × Al2O3A × Fe2O3tA × MnOA × MgOA × CaOA)]/ Na2OA }

ilr8KM = √ 8/9 × ln{[8√( SiO2A × TiO2A × Al2O3A × Fe2O3tA × MnOA × MgOA × CaOA × Na2OA)]/ K2OA }

ilr9PM = √ 9/10 × ln{[9√( SiO2A × TiO2A × Al2O3A × Fe2O3tA × MnOA × MgOA × CaOA × Na2OA × K2OA)]/ P2O5A }