APPENDIX C

Chapter 4

Supplementary Material for:

Geochemical analysis of Quaternary travertine deposits on the southeastern Colorado Plateau: Evaluation of travertine facies for paleohydrology and paleoenvironment studies

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Item DR1: Paleothermometry Calculations

Temperature calculations of the paleowater are based on the isotope fractionation equations by (1) Kim and O'Neil (1997), (2) Coplen (2007), and (3) Demény et al. (2010) for the system Calcite-H_2O:

(1) Kim and O'Neil: $1000 \ln\alpha = 18030/T - 32.42$,

(2) Coplen: $1000 \ln\alpha = 17400/T - 28.60$,

(3) Demény et al.: $1000 \ln\alpha = 17599/T - 29.64$,

where α is the fractionation factor and T the temperature in Kelvin. The fractionation factor α is calculated as follows (Sharp, 2007):

$$\alpha\ (\text{Calcite-}H_2O) = [(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)],$$

where $\delta^{18}O_c$ is the carbon isotope ratio of the calcite (travertine), and $\delta^{18}O_w$ the oxygen isotope ratio of the water. Substituting for α leads to modified fractionation equations:

(1) Kim and O'Neil (1997): $1000 \ln [(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)] = 18030/T - 32.42$,

(2) Coplen (2007): $1000 \ln [(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)] = 17400/T - 28.60$,

(3) Demény et al. (2010): $1000 \ln [(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)] = 17599/T - 29.64$,

which can be solved for T:

(1) $T = 18030 / [[(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)] + 32.42]$,

(2) $T = 17400 / [[(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)] + 28.60]$,

(3) $T = 17599 / [[(1000+\delta^{18}O_c) / (1000+ \delta^{18}O_w)] + 29.64]$,

where $\delta^{18}O_c$ is the measured carbon isotope ratio of the travertine converted into SMOW (Standard Mean Ocean Water) , and $\delta^{18}O_w$ the assumed oxygen isotope ratio of the paleo-water. Equations (1) – (3) can be solved for $\delta^{18}O_w$:

(1) $\delta^{18}O_w = e^{[[(-18.03/T)+0.032424+\ln(1000+ \delta 18Oc)]-1000]}$,

$$(2)\ \delta^{18}O_w = e^{[[(-17.4/T)+0.0286+\ln(1000+\ \delta18Oc)]-1000]},$$

$$(3)\ \delta^{18}O_w = e^{[[(-17.599/T)+0.02964+\ln(1000+\ \delta18Oc)]-1000]},$$

where $\delta^{18}O_c$ is the carbon isotope ratio of the travertine reported in SMOW and T is the assumed range of water temperature.