Calculator of precipitation temperature of biogenic phosphates based on the oxygen isotope composition (version 11) – notes

The calculator was developed by H. Wierzbowski[1] and is free to use for scientific purposes. A goal of this calculator is to compare precipitation temperatures of calcium carbonate calculated using different oxygen isotope temperature equations, which can be employed in palaeoenvironmental studies. Basically, problems of phosphate oxygen isotope temperatures may arise because of different analytical techniques or various reference $\delta^{18}O$ values. All appropriate corrections are used in the calculator

References and notes

1. Longinelli, A., Nuti, S., (1973a) Revised phosphate-water isotopic temperature scale. Earth and Planetary Science Letters 19, 373–376. *The equation (1) is established for phosphate admixtures separated from carbonate shells of molluscs in the 3.5-27°C temperature range. The authors have determined the temperature of ambient waters by analysis of oxygen isotope composition of $CaCO_3$ and using the calcite temperature equation of Craig (1965; see temperature calculator for calcium carbonate). This may be criticized as some shells composed of aragonite. Fish data presented by Longinelli and Nuti (1973b; Oxygen isotope measurements of phosphate from fish teeth and bones. Earth and Planetary Science Letters 20, 337–340) are within the range of temperatures and $\delta^{18}O_{phosphate}$ values calculated using the discussed equation. As the authors used $BiPO_4$ precipitation technique (with no reference value given) the data should be corrected for the reported difference of 1.4‰ in $\delta^{18}O$ values between NBS 120b reference measured using an older, $BiPO_4$ precipitation technique, and a newer, Ag_3PO_4 precipitation technique (cf. Lécuyer et al. 2013).*

   The corrected Longinelli and Nuti (1973a) equation is as follows:

   $$T(^oC) = 111.4 - 4.3*[(\delta^{18}O_{phosphate} - 1.4) - \delta^{18}O_{water}] \quad (1)$$

   where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale.

2. Kolodny, Y., Luz, B., Navon, O., (1983) Oxygen isotope variations in phosphate of biogenic apatites, I. Fish bone apatite – rechecking the rules of the game. Earth and Planetary science Letters, 64, 398–404. *The equation (2A) is established for fish skeletons in the 3-25.4°C temperature range. As the authors used $BiPO_4$ precipitation technique (with no reference value given) the data should be corrected for a reported difference of 1.4‰ in $\delta^{18}O$ values between NBS 120b reference measured using an older, $BiPO_4$ precipitation technique, and a newer, Ag_3PO_4 precipitation technique (cf. Lécuyer et al. 2013). Mathemetically modified, corrected version of this equation (2B) is presented in a study of Lécuyer et al. (2013).*

   The corrected Kolodny et al. (1983) equation (2A) is as follows:

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$T(^oC) = 113.3 - 4.38*[(\delta^{18}O_{phosphate} - 1.4) - \delta^{18}O_{water}]$ *(2A)*

where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale

The corrected Kolodny et al. (1983) equation presented by Lécuyer et al. (2013) is as follows:

$T(^oC) = 119.3 - 4.38*(\delta^{18}O_{phosphate} - \delta^{18}O_{water})$ *(2B)*

where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale

3. Lécuyer, C., Grandjean, P., Emig, C.C., (1996) Determination of oxygen isotope fractionation between water and phosphate from living lingulids: potential application to palaeoenvironmental studies. Palaeogeography, Palaeoclimatology, Palaeoecology 126, 101–108. *The authors have established a new temperature equation for modern lingulids in the 12-28°C temperature range. The authors use, accepted recently $\delta^{18}O$ value of NBS 120c of 21.7‰ VSMOW (cf. Lécuyer et al. 2013).*

$T(^oC) = 112.2 - 4.2*(\delta^{18}O_{phosphate} - \delta^{18}O_{water})$ *(3)*

where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale

4. Pucéat, E., Joachimski, M.M., Bouilloux, A., Monna, F., Bonin, A., Mortreuil, S., Morinière, P., Hénard, S., Mourin, J., Dera, G., Quesne, D., (2010) Revised phosphate-water fractionation equation reassessing paleotemperatures derived from biogenic apatite. Earth and Planetary Science Letters 298, 135–142. *The authors have established a new equation (4A) for teeth of reared fishes (eq. 1 in Pucéat et al. 2010) and presented another equation (4B) calculated using all published fish data (eq. 2 and 3 in Pucéat et al. 2010). In the latter compilation the authors have used their own data and published data of Longinelli and Nuti (1973b) and Kolodny et al. (1983) corrected for an assumed difference in $\delta^{18}O$ values of samples measured using an older, $BiPO_4$ precipitation technique and a newer, Ag_3PO_4 precipitation technique. As Pucéat et al. (2010) have used $\delta^{18}O$ value of NBS 120c reference of 22.6‰ VSMOW, their equations should be normalized to the NBS 120c values of 21.7‰ VSMOW, which is accepted recently (cf. Lécuyer et al. 2013). The latter calibration is, however, predicted in the mathematical formula of the second equation presented by in Pucéat et al. (2010).*

The new fish equation of Pucéat et al. (2010) corrected for the NBS 120c values of 21.7‰ is as follows:

$T(^oC) = 124.6 - 4.52*[(\delta^{18}O_{phosphate} + 0.9) - \delta^{18}O_{water}]$ *(4A)*

where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale

The equation of Pucéat et al. (2010) for all published data with applied corrected for the NBS 120c values of 21.7‰ is as follows:

$$T(^{o}C) = 118.7 - 4.22*[(\delta^{18}O_{phosphate} + 0.9) - \delta^{18}O_{water}] \quad (4B)$$

where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale

5. Lécuyer, C., Amiot, R., Touzeau, A., Trotter, J., (2013) Calibration of the phosphate $\delta^{18}O$ thermometer with carbonate-water oxygen isotope fractionation equations. Chemical Geology 347, 217–226. *The authors have established a new equation (5) based on published data from lingulids (after Lécuyer et al. 1996) and fishes (after Picard et al. 1998, Geolgy 26, 975–978) for the 12-28°C temperature range. The authors have used recently accepted $\delta^{18}O$ value of NBS 120c of 21.7‰ VSMOW and claim, based on comparison of temperatures calculated using various equations, that that their equation yields the most consistent phosphate-carbonate temperature estimates.*

$$T(^{o}C) = 117.4 - 4.5*(\delta^{18}O_{phosphate} - \delta^{18}O_{water}) \quad (5)$$

where $\delta^{18}O_{phosphate}$ is the oxygen isotope composition of carbonate on the VSMOW scale and $\delta^{18}O_{water}$ is the oxygen isotope composition of water on the VSMOW scale