Compressional behavior of the aragonite-structure carbonates to 6 GPa.

Supplementary Material

Isaac Vidal-Daza[*,1] *Antonio Sánchez-Navas*[2,3] *and Alfonso Hernández-Laguna*[3]

[1]Grupo de Modelización y Diseño Molecular, Facultad de Ciencias Universidad de Granada 18071 Granada Spain.

[2]Departamento de Mineralogía y Petrología Facultad de Ciencias Universidad de Granada 18071 Granada Spain

[3]Instituto Andaluz de Ciencias de la Tierra (CSIC-UGR) Av. de las Palmeras 4 18100 Armilla Granada Spain.

Table S1. Cell parameter values (Å), linear moduli (GPa) and first derivative with respect to pressure of the bulk modulus of aragonite-structure carbonates.

	Arago.	Arago. exp[2]	Stront.	Stront. exp	Ceruss.	Withe.	With. exp
a_0	4.9522	4.959	5.1146	5.085[3]; 5.08577[54]	5.2179	5.3206	5.288[3]; 5.316[6]
K_{0a}	344.1	344.7	234.0	115[3]; 322.2[5]	271.5	306	91[3]; 369[6]
K'_{0a}	8.6	8.0	27.1	7.2[5]	28.3	99	26[6]
K''_{0a}	-0.26	-0.21	-7.2	-0.2[5]	-6.8	-89	-4[6]
b_0	7.8863	7.97	8.3735	8.441[3]; 8.4416[54]	8.52028	-[1]	8.943[3] 8.892[6]
K_{0b}	259.5	181.2	283.8	78; 231.3[5]	383	-	84[3]; -
K'_{0b}	8.7	11.5	17.7	4.9[5]	73	-	-
K''_{0b}	-0.35	-1.1	-2.2	-0.1	-38	-	-
c_0	5.6703	5.741	5.9522	6.026[3]; 6.0251[54]	6.1122	6.3168	6.452[3]; 6.428[6]
K_{0c}	153.9	131.1	105	34[3]; 103.5[5]	82.5	57.9	22[3]; 65.7[6]
K'_{0c}	2.3	3.9	1.5	3.7[5]	1.5	1.4	1.0[6]
K''_{0c}	-0.10	-0.08	-0.21	-0.1[5]	-0.28	-0.42	-0.4[6]

[1] No values because of the b softening at 3 GPa.

[2] From Palaich's et al. (2016) data to 6 GPa.

[3] From Wang et al. (2015) (Wang15a) in the silicon oil media.

[4] Cell parameter optimized in either BM3 or BM2.

[5] From Wang et al. (2015) in the methanol and ethanol media.

[6] Results from Holl et al. (2000).

1 Deduction of equation (13) of the main manuscript

Following Anderson and Nafe (Anderson and Nafe 1965) we can start with the identity:

$$\frac{dK}{dV} = \frac{dK}{dP}\frac{dP}{dV} \tag{1}$$

where K is the bulk modulus of a crystal, V is the cell volume of the crystal, and P is the pressure.

$$K = -V\frac{dP}{dV} \Rightarrow \frac{dP}{dV} = -\frac{K}{V} \tag{2}$$

Eq. 2 is introduced in Eq. 1

$$\frac{dK}{dV} = -\frac{dK}{dP}\frac{K}{V} \tag{3}$$

$\frac{dK}{dP} = K'$ the first derivative of the bulk modulus with respect to pressure.
By arranging Eq. 3:

$$\frac{dK}{K} = -K'\frac{dV}{V} \tag{4}$$

If this K' is independent of the volume, Eq. 4 can easily integrate giving the Anderson and Nafe's equation:

$$\ln K = -K' \ln v + C \tag{5}$$

Where C is the integration constant. However, if K' is dependent of the volume, K' can be expanded in Taylor's series, such as:

$$K' = -K'_0 + \frac{dK'}{dV}(V - V_0) + \frac{d^2K'}{dV^2}(V - V_0)^2 + \cdots \tag{6}$$

By introducing the two first terms of the second member of Eq. 6 in Eq. 4 results:

$$\int \frac{dK}{K} = -\int [K'_0 + \frac{dK'}{dV}(V - V_0)]\frac{dV}{V} = -\int K'_0\frac{dV}{V} - \int \frac{dK'}{dV}(V - V_0)\frac{dV}{V} = -K_0 \ln V + C_1 - K'\frac{V - V_0}{V} + C_2 \tag{7}$$

Which result:

$$\ln K = -K'_0 \ln V - K'(\frac{V - V_0}{V}) + C \tag{8}$$

This equation can be consider as an extension of the Anderson and Nafe's equation (Anderson and Nafe 1965), where their equation is the first term of the second member, and the extension is the second term plus C, which the integration constant coming from the addition of the different integration constants Eq. 7.

References

Anderson OL, Nafe JE (1965) The bulk modulus-volume relationship for oxide compounds and related geophysical problems. Journal of Geophysical Research (1896-1977) 70(16):3951–3963, https://dx.doi.org/https://doi.org/10.1029/JZ070i016p03951, URL https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/JZ070i016p03951, https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/JZ070i016p03951