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addenda and errata

Lattice constants and thermal expansion of H_2O and D_2O Ice I*h* between 10 and 265 K. Addendum

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In a previous paper we reported the lattice constants and thermal expansion of normal and deuterated ice I*h* [Röttger *et al.* (1994). *Acta Cryst.* B**50**, 644–648]. Synchrotron X-ray powder diffraction data were used to obtain the lattice constants and unit-cell volumes of H_2O and D_2O ice I*h* in the temperature range 15–265 K. A polynomial expression was given for the unit-cell volumes. It turns out that the coefficients quoted have an insufficient number of digits to faithfully reproduce the volume cell data. Here we provide a table with more significant digits. Moreover, we also provide the coefficients of a polynomial fit to the previously published *a* and *c* lattice constants of normal and deuterated ice I*h* for the same temperature range.

In a previous paper we reported the lattice constants and thermal expansion of normal and deuterated ice I*h* (Röttger *et al.*, 1994). Synchrotron X-ray powder diffraction data were used to obtain the lattice constants and unit-cell volumes of H_2O and D_2O ice I*h* in the temperature range 15–265 K. A polynomial expression was given for the unit-cell volumes. It turns out that the coefficients quoted have an insufficient number of digits to faithfully reproduce the volume cell data. This is due to the large correlations amongst the terms of even as well as uneven order. Here we provide a table with more significant digits and also correct one rounding error for the A_3 term of the H_2O unit-cell volume. Moreover, we also provide the coefficients of a polynomial fit to the previously published *a* and *c* lattice constants of normal and deuterated ice I*h* for the same temperature range. In Table 1 these coefficients are given together with the quality of the fit. The database is identical to that given in Röttger *et al.* (1994). The coefficients A_1 and A_2 were set to zero as the thermal expansivity and its temperature derivative are assumed to be 0 at $T = 0$ K. Under this assumption the validity of the polynomial expressions is from 0 to 265 K. Finally, we like to recall that a many-term polynomial expression was adopted to faithfully represent the measured data and not because there is a particular meaning in the various higher-order terms. We indicate that other approaches could be chosen based on various empirical quasi-harmonic approximations (Reeber & Wang, 1996; Wang & Reeber, 1995) with a different set of parameters; the validity of these approximations for the ice I*h* case remains, however, to be proven and will not be attempted here. In concluding we note that the marked isotopic difference of lattice constants between deuterated and normal ice I*h* so clearly established by our data is still far from being understood (Herrero & Ramírez, 2011).

References

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Table 1
Coefficients of the polynomial expression $V_{\text{unit cell}}(T) = A_0 + A_1T + A_2T^2 + A_3T^3 \ldots + A_8T^8$ and $\mathbf{a}(T)$, $\mathbf{c}(T) = A_0 + A_1T + A_2T^2 + A_3T^3 \ldots + A_8T^8$.

Uncertainties corresponding to the 90% confidence level are given in brackets and refer to the last digits of the coefficients (ignoring any additional digits given as subscripts in the case of A_0). The quality of fit is given as χ^2.

	Unit-cell volume H_2O ice I*h*	Lattice constant **a** H_2O ice I*h*	Lattice constant **c** H_2O ice I*h*	Unit cell volume D_2O ice I*h*	Lattice constant **a** D_2O ice I*h*	Lattice constant **c** D_2O ice I*h*
A_0	128.2147 (159)	4.4969_{15} (2)	7.3211_{25} (3)	128.3316 (151)	4.4982_{8} (2)	7.3233_{6} (6)
$A_1 = A_2$	0	0	0	0	0	0
A_3	-1.3152 (2643) $\times 10^{-6}$	-1.9790 (3205) $\times 10^{-8}$	-2.4944 (6146) $\times 10^{-8}$	-2.2616 (6547) $\times 10^{-6}$	-3.9099 (7361) $\times 10^{-8}$	-3.0567 (1.4264) $\times 10^{-8}$
A_4	2.4837 (5228) $\times 10^{-8}$	3.8958 (6356) $\times 10^{-10}$	4.6735 (1.2806) $\times 10^{-10}$	5.1581 (1.7731) $\times 10^{-8}$	9.7883 (2.1911) $\times 10^{-10}$	5.9033 (2.9651) $\times 10^{-10}$
A_5	-1.6064 (3876) $\times 10^{-10}$	-2.6930 (4820) $\times 10^{-12}$	-2.9799 (9966) $\times 10^{-12}$	-4.5811 (1.9116) $\times 10^{-10}$	-9.7393 (2.5879) $\times 10^{-12}$	-3.9203 (2.3100) $\times 10^{-12}$
A_6	4.6097 (1.2625) $\times 10^{-13}$	8.2861 (1.6256) $\times 10^{-15}$	8.3902 (3.4003) $\times 10^{-15}$	2.0890 (1.0144) $\times 10^{-12}$	4.9329 (1.4896) $\times 10^{-14}$	1.1541 (7936) $\times 10^{-14}$
A_7	-4.9661 (1.5196) $\times 10^{-16}$	-9.5759 (2.0415) $\times 10^{-18}$	-8.8400 (4.2799) $\times 10^{-18}$	-4.8591 (2.6388) $\times 10^{-15}$	-1.2573 (4168) $\times 10^{-16}$	-1.2751 (1.0119) $\times 10^{-17}$
A_8	0	0	0	4.5747 (2.6900) $\times 10^{-1}$	1.2798 (4546) $\times 10^{-19}$	0
χ^2	6.91	8.84	9.36	6.12	10.28	3.97

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