Table M19-001. H_2O (ice). Fractional coordinates, anisotropic and anharmonic temperature parameters of phase Ih by X-ray diffraction experiment [90Got]. T = 243 K. b_{ij} is defined by Eq. (b) in Introduction. Anharmonic correction was made by using Gram-Charlier series expansion of the temperature factor: $T_{GC}(\boldsymbol{g}) = T_h(\boldsymbol{g})[1 + \{(2\pi i)^3/3!\} C_{pqr} g_p g_q g_r + \{(2\pi i)^4/4!\} D_{pqrs} g_p g_q g_r g_s]$, where $T_h(\boldsymbol{g})$ is a harmonic temperature factor, $\boldsymbol{g}$ the reciprocal lattice vector, and C_{pqr} and D_{pqrs} are the third and fourth symmetric polar tensors, respectively. Figures in parentheses indicate standard deviations on last digits.

	Harmonic approximation	Anharmonic analysis
O		
z	0.06226(8)	0.0618(3)
b_{11}	0.0603(5)	0.0629(4)
b_{33}	0.0172(1)	0.0186(4)
C_{111}		$1.8(4) \cdot 10^{-5}$
C_{113}		$0.1(3) \cdot 10^{-5}$
C_{333}		$-1.6(6) \cdot 10^{-6}$
D_{1111}		$1.3(7) \cdot 10^{-6}$
D_{1113}		$4(12) \cdot 10^{-7}$
D_{1133}		$11(4) \cdot 10^{-7}$
D_{3333}		$3(7) \cdot 10^{-7}$
H1		
z	0.178(3)	0.173(4)
b_{11}	0.051(10)	0.039(10)
b_{33}	0.0056(29)	0.013(3)
H2		
x	0.439(3)	0.437(2)
y	0.878(4)	0.873(4)
z	0.020(2)	0.024(2)
b_{11}	0.048(7)	0.037(5)
b_{22}	0.036(10)	0.037(10)
b_{33}	0.016(3)	0.016(4)
b_{13}	0.019(9)	–0.009(9)

where O: $x = 1/3, y = 2/3$
$b_{11} = b_{22} = 2 \cdot b_{12}$, $b_{13} = b_{23} = 0$
$C_{111} = -1 \cdot C_{222} = 2 \cdot C_{112} = -2 \cdot C_{122}$
$C_{113} = C_{223} = 2 \cdot C_{123}$, $C_{133} = C_{233} = 0$
$D_{1111} = D_{2222} = 2 \cdot D_{1112} = 2 \cdot D_{1122}$
$D_{1113} = -1 \cdot D_{2223} = 2 \cdot D_{1123} = -2 \cdot D_{1223}$
$D_{1133} = D_{2233} = 2 \cdot D_{1233}$, $D_{1333} = D_{2333} = 0$

where H1: $x = 1/3, y = 2/3$
$b_{11} = b_{22} = 2 \cdot b_{12}$, $b_{13} = b_{23} = 0$

where H2: $b_{22} = 2 \cdot b_{12}$, $b_{13} = 2 \cdot b_{23}$

Table M19-002. H_2O (ice). Structure of phase Ih by X-ray diffraction [90Got] and neutron diffraction [83Kuh]. The root-mean-square displacements [Å], interatomic distances [Å] and bond angles [°]. See Table M19-001.

	X-ray diffraction [90Got] T = 243 K		Neutron diffraction [83Kuh] T = 223 K
	Harmonic approximation	Anharmonic analysis	
O ∥ c	0.2167(9) Å	0.225(2) Å	0.2069(14) Å
O ⊥ c	0.2159(9) Å	0.220(2) Å	0.2096(10) Å
H1 ∥ c	0.12(3) Å	0.19(2) Å	0.2115(41) Å
H1 ⊥ c	0.20(2) Å	0.17(2) Å	0.2409(28) Å
H2 ∥ a	0.19(1) Å	0.17(1) Å	0.2421(23) Å
H2 ⊥ a	0.21(2) Å	0.21(2) Å	0.2407(27) Å
O–O′	2.7583(8) Å	2.765(3) Å	2.759(2) Å
O–O″	2.7604(8) Å	2.758(3) Å	2.760(1) Å
O–H1	0.85(2) Å	0.82(3) Å	1.008(4) Å
O–H2	0.88(2) Å	0.85(2) Å	1.004(2) Å
∠O′–O–O″	109.35(2)°	109.23(10)°	109.35(4)°
∠O″–O–O‴	109.59(2)°	109.72(10)°	109.60(5)°
∠H1–O–H2	110(2)°	109(2)°	109.44(27)°
∠H2–O–H2	108(2)°	110(2)°	109.50(27)°

The bonds O–H1 and O–O′ are parallel to the c axis and other bonds O–H2, O–O″, and O–O‴ are oblique to the c axis.

Table M19-003. D_2O (deuterated ice). Structure of phase Ih [85Lea]. Lattice parameters, fractional coordinates, and temperature parameters. (a) Neutron diffraction of single crystal D_2O at 123 K [57Pet]. (b) Neutron powder diffraction of KOD-doped D_2O at 121 K [85Lea]. B_{ij} is defined by Eq. (a) in Introduction.

	(a)	(b)
a [Å]	4.489	4.5040(1)
c [Å]	7.327	7.3337(2)
z (O)	0.0620(4)	0.0636(7)
z (D1)	0.1980(7)	0.1993(4)
x (D2)	0.4545(9)	0.4532(3)
z (D2)	0.0172(4)	0.0164(8)
B_{11} (O) [Å^2]	1.53(11)	1.50(12)
B_{33} (O) [Å^2]	1.48(10)	2.03(21)
B_{11} (D1) [Å^2]	2.41(13)	2.71(9)
B_{33} (D1) [Å^2]	1.81(12)	0.81(26)
B_{11} (D2) [Å^2]	2.29(21)	2.27(9)
B_{22} (D2) [Å^2]	1.85(12)	1.90(41)
B_{33} (D2) [Å^2]	2.43(10)	2.46(26)
B_{23} (D2) [Å^2]	0.96(36)	–0.48(35)

Table M19-004. D_2O (deuterated ice). Structure of phase XI by neutron powder diffraction of KOD-doped D_2O [85Lea]. T = 5 K. Lattice parameter: a = 4.5019(5) Å, b = 7.7978(8) Å, c = 7.3280(2) Å. The isotropic temperature parameter B is defined by Eq. (e) in Introduction.

	O1	O2	D1	D2	D3
x	0.0000	0.5000	0.0000	0.0000	0.6766(19)
y	0.6648(18)	0.8255(21)	0.6636(29)	0.5363(14)	–0.2252(13)
z	0.0631(2)	–0.0631	0.1963(4)	0.0183(3)	–0.0183
B [Å^2]	0.74(18)	1.06(20)	1.54(9)	1.53(5)	1.53