**Raman Spectroscopy of Phase Transitions in the H-Sublattice of H₂O-Ices**

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**Introduction:**

• In total, 20 different crystalline structures of water ice have been discovered [1,2,4].
• One reason for that diversity is the existence of both one H-disordered high-temperature phase and one H-ordered low-temperature phase for most oxygen lattice.
• In 2017, an alternatively H-ordered proxy of ice VI additionally to ice XV was discovered – ice XIX [1].
• Its structure was resolved in 2020 and the unit cell has twice the size of that of ice VI & XV.
• That is the first known example of alternative H-ordering.

**Goal:**

• Determination of mechanism and kinetics of the first known H-order-order transition in ice chemistry.
• Investigation of potential other examples for alternative H-ordering.

**Method:**

• **Raman-Spectroscopy** is a method in order to detect inter- and intramolecular vibrations of a sample by a special scattering effect – Stokes scattering.
• After undergoing Stokes scattering the energy of the scattered light is reduced by the vibrational energy.
• These differences can only be measured if the inciting light is monochromatic. In these experiments a laser of 521 nm wavelength are used.
• As inter- and intramolecular vibrations get detected, Raman spectroscopy is especially sensitive for structural differences in the H-sublattice.

**Results:**

• Raman spectra of ice VI, XV and XIX are distinguishable from each other.
• The complete H-order-order transition can be traced through Raman spectroscopy.

- Ice XIX is heated to different temperatures and Raman spectra are recorded there isothermally. (top, right)
- The ice XIX and ice XV-fraction are calculated by superpositions. (top, middle)
- These fractions can be plotted against their transformation time. Through Avrami fits parameters of interest such as the rate constant \( k \) and the Avrami exponent \( n \) can be derived. (top, left)

**Sources:**

[6] bwtek.com/raman-theory-of-raman-scattering/Fig. B4

**Activation energy for ice XIX -> XV:**

\[ E_A = 23 \text{ kJ/mol} \]