High Pressure Stability of Hydrogen Bonded Crystal of Squaric Acid: H/D Isotope Effect

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Background:
- Hydrogen bonding (HB) plays a key role in determining the structure and properties of many molecular systems
- Squaric acid (SQA) is a prototypical HB molecular crystal
- Behavior of HB not well understood under high pressure
- Previous work on SQA revealed that structural stability of this crystal is governed by changes in the HB
- H/D isotope effect (substitution of hydrogen with deuterium) is often used to gain insight into the HB

Objectives:
- Use the H/D isotope effect to further examine the role of hydrogen bonding in structural stability of SQA crystal
- Is deuterated SQA (D-SQA) structure more stable under high pressure than H-SQA (positive Ubbelohde effect)?

Experimental Approach:
- Refluxing of H-SQA with D₂O and growing single crystals of D-SQA

Summary/Conclusions:
- Performed first high pressure measurements on D-SQA up to 22 GPa
- D/H isotope effect further stabilizes the structure of SQA under high pressure

References:

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