

# Reactivity in crystalline and amorphous high-pressure ices



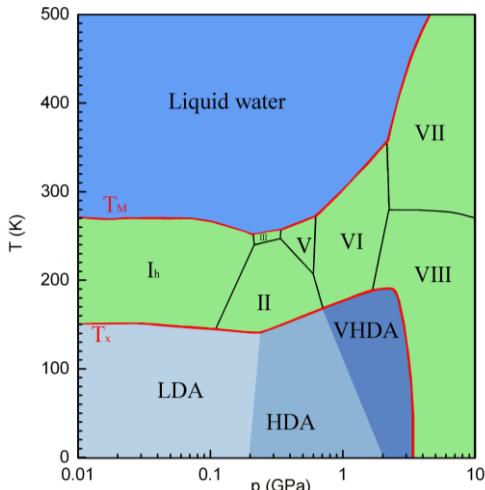
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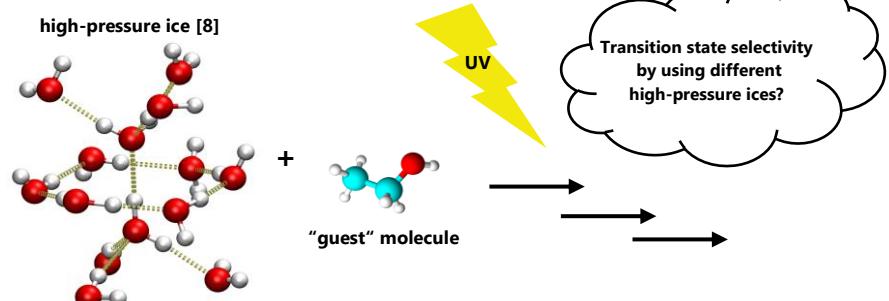
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## The exceptional features of water



Water is considered to be anomalous in many aspects. Having two hydrogen-donor and two hydrogen-acceptor sites in each molecule, the versatility of the hydrogen bond network in water is exceptional [2]. This fact becomes obvious in view of water's particularly rich state diagram especially at low temperatures and high pressures. To date, the structures of 18 crystalline and 3 distinct amorphous ices [3] are known. Nevertheless, knowledge of their chemical reactivity is limited. While some photochemical reactions have been scrutinised in low-pressure ices [4-7], similar reactions in high-pressure ices have not been studied yet. High-pressure ices are most likely more reactive than low-pressure ices because of their distorted hydrogen bond networks. It is therefore the aim of the present PhD project to explore the photochemical reactivity in crystalline and amorphous ices upon ultraviolet (UV) irradiation.



## Key steps of the project

1. Spectroscopic characterisation of high-pressure ices in UV-VIS-NIR range

2. UV-Irradiation experiments, monitoring the solid phase by IR, Raman

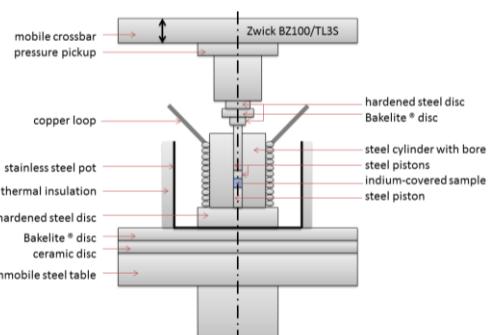
3. UV-Irradiation experiments, monitoring the gas phase by CP-FTMW

University of Innsbruck (Loerting Lab)

DESY (Schnell Lab)

## Experimental

High-pressure ices are prepared using the piston cylinder set-up established in the Loerting Lab (right). Regarding the UV/VIS and NIR characterisation of high-pressure poly(a)morphs the utilisation of spectrometers of the desired spectral range seems straightforward. However, the necessity of keeping the ice samples at temperatures  $< 100$  K during spectroscopic measurements without condensation of ordinary hexagonal ice is far from trivial. To overcome these problems, powdered ice samples will be cooled by liquid nitrogen during NIR and UV/VIS measurements in diffuse reflection mode. In Step 2 of this project, an IR spectroscopy setup including a Varian 3100 FT-IR spectrometer operating in transmission mode will be used. It is the aim to achieve UV-irradiation experiments with *in situ* FT-IR and *ex situ* XRD characterisation of the high-pressure ice samples. In order to study the gas phase during radiation experiments, a microwave spectroscopy (CP-FTMW) setup in the Schnell Lab at DESY (Hamburg) will be employed. This method detects rotational transitions of polar molecules in the gas phase. Since rotational spectra depend on the moments of inertia of the molecules, structural isomers, conformers, and even isotopologues have unique rotational spectra and can be unambiguously differentiated. As a result, CP-FTMW is uniquely mixture sensitive.



Schematic depiction of the high-pressure piston cylinder setup used in the Loerting lab [9].

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