# 2. Theory and methods

## 2.1. IR Spectroscopy

## 2.2. Neutron Scattering

### 2.2.1. Scattering theory

### 2.2.2. NIMROD Instrument

### 2.2.3. Limitations

## 2.3. Acoustic Levitation

## 2.4. The Portable Astrochemistry Chamber

The Portable Astrochemistry Chamber (PAC), shown in Figure 1, has been designed by Anita Dawes in 2003 (citation Anita) in order to simulate the prevailing conditions in molecular clouds, where ice is known to grow from the condensation of atomic species on the cold surface of sub-µm dust grains (citation). It is now a well-established experimental setup that can achieve temperatures as low as 20K and Ultra High Vacuum (UHV) of 10-10 mbar, while remaining transportable. It has been used so far for various Astrochemistry experiments (citations), including work at large scale facilities (Aarhus – Danmark – citation Rachel – Anita - excitons)

### 2.4.1. Setup description

Diagram

Description automatically generated

**Figure 1**: Photograph of the PAC highlighting the main experimental components. Colors refereed to the experimental steps and will be further described in the text: green have to do with setting up the experimental conditions in the main chamber; blue point out the gas dosing lines required and subsequent steps for growing the ice and finally red have to do with data acquisition.

**The main chamber**

The main chamber is a spherical cube (Kimball Physics MCF275-SC600-A) whose inner diameter is 66 mm, featuring six ConFlat (CF) 40 flanges on each face. At the center of the chamber lie the substrate onto which the ice is deposited. The substrate is a zinc selenide (ZnSe) spherical Infrared (IR) window, selected to maximize the transmission in the range 4000 – 800 cm-1 (refer to background figure), hold by an oxygen free high conductivity copper frame (Goodfellow) directly attached to the cold head of a two-stage closed cycled helium cryostat (Sumitomo HC-202B), that is supplied by a helium compressor (Sumitomo HC-4E). The cryostat is inserted in a stainless-steel extension piece attached to a rotary feedthrough (MDC ERMTG 275) and connected to the top of the chamber via a CF100-to-CF40 adapter, allowing the substrate a 90° rotation resulting in two possible configurations (deposition and scan). The substrate temperature is monitored via a silicon diode temperature sensor (Lake Shore Cryosensors DT-670B-SD) and adjusted by the use of a Kapton flexible resistive heater (Omega), both connected via a 10-pin CF16 electrical feedthrough to an external Proportional Integral Derivative (PID) temperature controller, with respective settings of ? (worth showing a temperature ramp?).

The main chamber is pumped by a turbomolecular pump (Leybold TURBOVAC TMP 151) attached at the bottom by a CF40-to-CF100 adapter and backed by a two-stage oil rotary vane pump (Leybold TRIVAC D4B). The chamber pressure is monitored using a combination gauge (Leybold IONIVAC ITR 90) with a minimum reading pressure of 5 × 10-10 mbar. Base temperature and pressure of 20K and 10-10 mbar can be achieved in the main chamber (with little variation resulting from the experiment history), that are relevant to molecular clouds conditions.

**The Gas Dosing Line**

Figure in prep

Once the best vacuum pressure is achieved in the main chamber, the ice is grown by physical vapor deposition onto the substrate, set at the desired temperature. Two sets of experiments will be achieved with the PAC, the first one using only water (Chapter 3) and the second involving a binary mixture of water and ethane (C2H6) (Chapter 4). The gas dosing line is made of 6 mm stainless steel tubing connected downstream to a two-stage oil rotary vane pump (Leybold TRIVAC D4B), and upstream to the gas mixing chamber, a T piece with a volume of ? that act as a mixing reservoir. 10 ml of distilled liquid water is contained in a sealed test tube, attached via (forgot the name of this connection) followed by an on/off valve (V1) and connected to the gas line

### 2.4.2. Experimental procedure

### 2.4.3. Data acquisition

OMNIC

**Ice thickness Calculation**

### 2.4.4. Data Reduction

Following acquisition, the data is transferred via USB and processed using self-developed python code. Jupiter Notebook has been chosen as a development console for its readiness and ease of use.

3 notebooks have been produced for every step of the data reduction pipeline highlighted in Figure X

DR1

The data is segmented in 3 range 400:2800; 2800:1900; 1900:800 corresponding to the Oh stretching modes,

DR2

No investigation into background signature Data split in 3 ranges for better reliability

### 2.4.5. Data Processing