# Experimental report

23/11/2015

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| **Proposal:** | **6-05-961** | **Council:** | 10/2014 |
| **Title:** | The connection between fast and slow dynamics in glass-forming liquids: a test of the "isomorph theory" of simple liquids | | |
| **Research area:** | Soft condensed matter | | |

**This proposal is a resubmission of 6-05-943**

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| **Main proposer:** | **Kristine NISS** |
| **Experimental team:** | Henriette Wase HANSEN<br>Kristine NISS<br>Alejandro SANZ<br>Simone CAPACCIOLI<br>GAIA CIAMPALINI |
| **Local contacts:** | Bernhard FRICK<br>Judith PETERS |

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| **Samples:** | Dibutylphthalate ($C_{16}H_{22}O_4$)<br>Dipropylene glycol ($C_6H_{14}O_3$) |

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| IN16B | 7 | 7 | 30/06/2015 | 07/07/2015 |
| IN13 | 7 | 7 | 20/07/2015 | 27/07/2015 |

## Abstract:

The molecules in a liquid close to the glass transition move on a range of timescales. Vibrations take place on the picosecond timescale while relaxations can be as slow as minutes or hours. It has several times been suggested that there is a close connection between the fast and slow dynamics, even though they differ in time scales by ten or more orders of magnitude. The recently developed isomorph theory rationalizes this connection. The aim of this experiment is to measure fast dynamics (~ nanosecond) at different state points (T-P) along lines in the phase diagram where the slow alpha relaxation is constant (so called isochrones), because the isomorph theory predicts that the fast relaxation should be invariant along these lines. The experiment requires measurements at elevated pressure, which is in itself interesting because relatively little INS/QENS high pressure data is available on glass-forming liquids. Two prototypical liquids will be studied: a van der Waals molecular liquid and an hydrogen bonded one, showing opposite trends for the pressure dependance of fragility.

# Experimental report, exp. no. 6-05-961, IN16b and IN13

July 2015

Glass and Time, Roskilde University

The aim of this experiment was to test the isomorph theory by measuring the fast dynamics along isochrones, which are lines in the TP-diagram with constant relaxation time, along which the dynamics is invariant according to the isomorph theory. Isochrones are studied on IN16b and IN13, i.e. with two different time resolutions, by varying temperature and pressure. The isomorph theory is only predicted to hold for strongly correlating liquids, e.g. van der Waals bonded liquids, here represented by isopropyl benzene (cumene), and to break down for hydrogen bonded liquids, tested with dipropylene glycol (DPG).

Both samples, cumene and DPG, were studied at IN16b, while only cumene was used for the second beamtime on IN13. On IN16b, both samples were studied using the fixed window scan (FWS) technique. Temperature and pressure scans were performed to explore the PT-phase diagram and to find state points along an isochrone where to do full spectra.

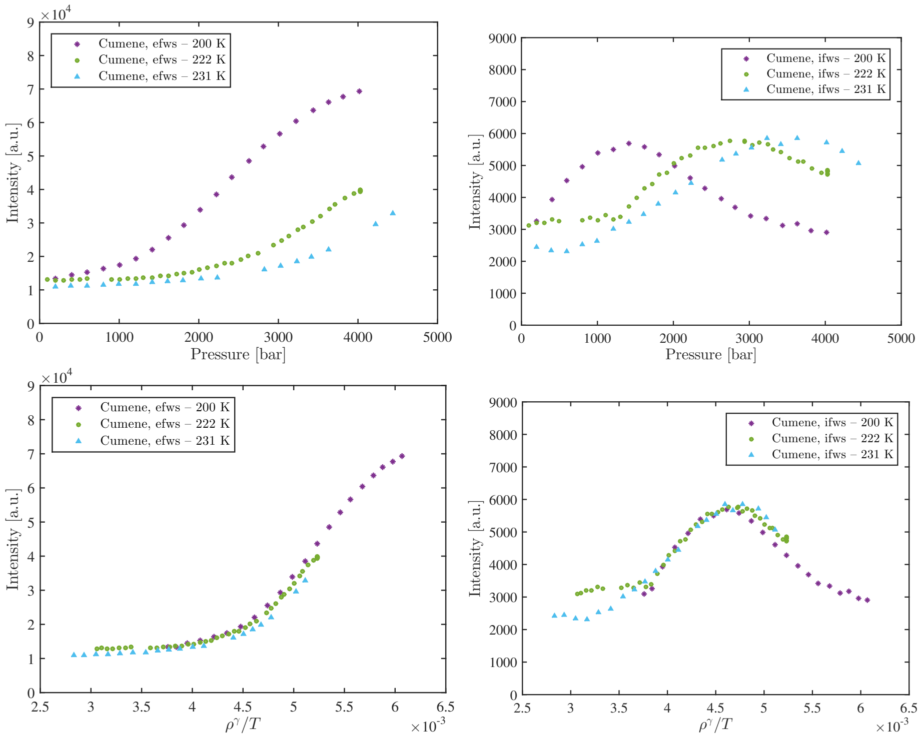

Figure 1: Top: Pressure scan on IN16b. Bottom: Density scaling on data. Summed over $Q$.

In Figure 1 and 2, from IN16b and IN13, respectively, we see that density scaling makes the data collapse nicely. The parameter $\gamma$ was found from viscosity data on cumene. In Figure 3, we see the consequence of the isomorph prediction

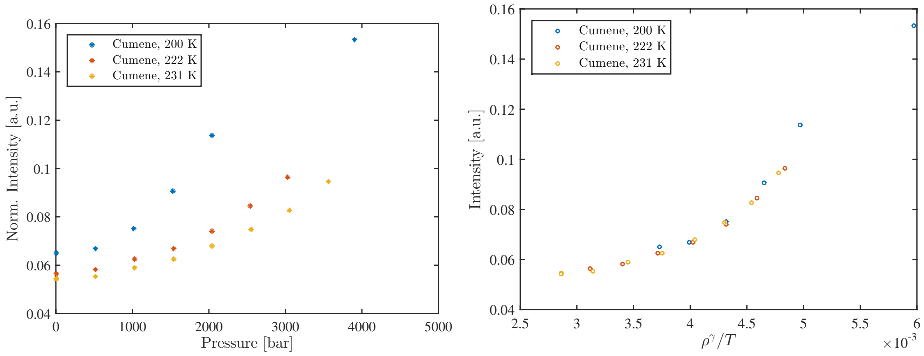

Figure 2: Left: Pressure scan on IN13. Right: Density scaling on data. Summed over $Q$.

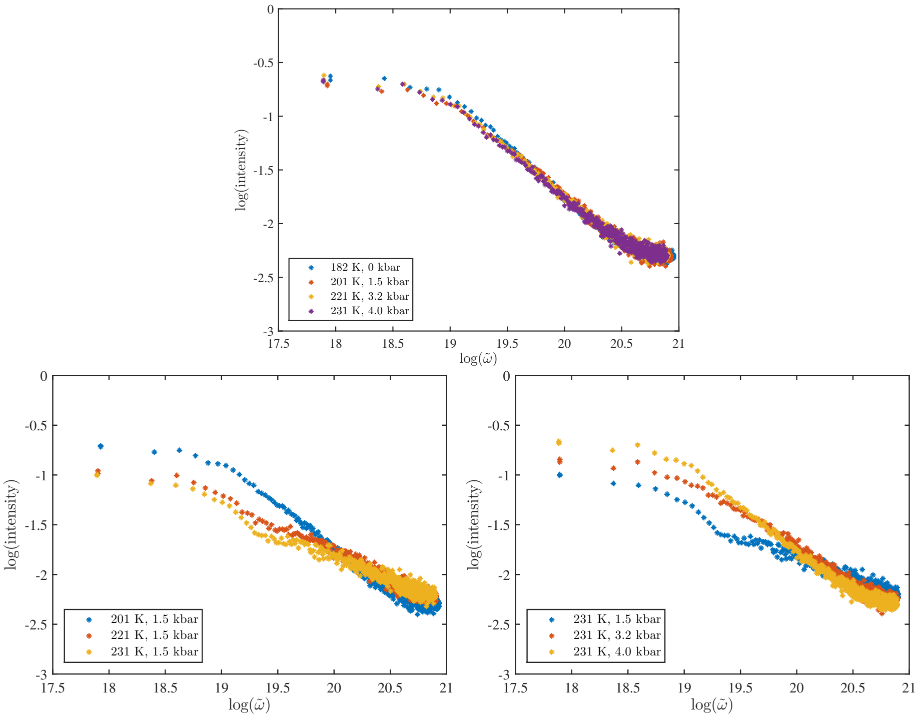

Figure 3: QENS on cumene on IN16b. Top: Isochrone. Bottom: Isobar and isotherm. Summed over $Q$.

for a van der Waals bonded liquid; dynamics are constant along an isochrone, here compared with dynamics along an isobar and an isotherm. From this point of view, a very successful experiment.

However, unfortunately, we see almost no effect of pressure on the DPG sample. It is clear from the FWS data on DPG (Fig. 4) that something is not right. It seems there is no effect in pressure at all before reaching a pressure of 2 kbar. This is very different from the cumene data (Fig. 1), where the effect of pressure and the temperature dependence of this effect are clear just above ambient pressure.

We do not know exactly what caused this lack of pressure effect for our second sample on IN16b. We have discussed back and forth with the beamline scientists and the sample environment team, and although everyone has been extremely helpful in trying to solve this puzzle, we have not been able to explain it. Unfortunately, this means that we will not be able to use the temperature scans, pressure scans or QENS spectra on DPG.

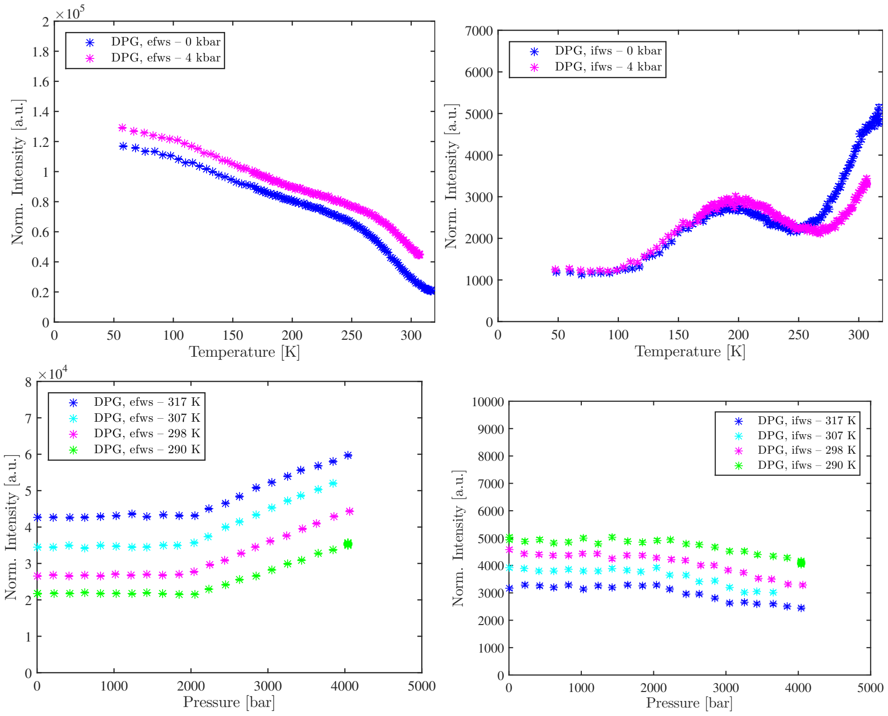

Figure 4: Temperature (top) and pressure (bottom) scans on IN16b on DPG. Summed over $Q$.

So overall, a very successful first part of the experiment, which for a large part was due to the very skilled and helpful beamline scientists and sample environment team that we have had the pleasure of working with, but unfortunately not successful for the second part.