KBr and Ceria Model Run for a Good Fit

Date: 2023-02-21
Tags: Reference | high pressure | DRFITS | KBr | CeO2 powder
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Goal :

To run an experiment for both KBr and CeO_2 under the same conditions on the same day to try and get the absolute best fit for KBr reference data (Needed for the Mathematica script).

Procedure :

Carbonyl trap heated at 450 °C for 45 min
Liquid N2 detector cooled at 08:30
Water trap cooled --> re-cool after every 30 minutes.

Initial start with KBr start time 09:00 am
Run background before heating in O2 atmosphere LC0043.0

Heater started at 09:05 am --> Heating to 225 °C for 2 hours
Heater switched off at 11:05 am
Cooling down to 28 °C
Finished cooling 11:56

Background run after heating LC0043.1

Measurment parameters:
Signal intensity:3106
Resolution: 2 cm-1
Scan rate for background: 512
Scan rate for repeated spectra: 8

Measurments at 0.2 bar of CO: (Additional note: flow here at 0.2 bar is 101 ml/min)
LC0043.0000-0099

Measurments at 0.5 bar of CO:
LC0043.0100-0199

Measurments at 1.0 bar of CO:
LC0043.0200-0299

Experiment stopped and spectrometer filled with LN_2

Start O_2 flow and run background LC0043.2 (Now Ceria)
Heat sample to 750 °C for 2 hours (Started at 12:40)
Cooling down started at 14:20
cooling to 28 °C
Time at 28 °C 15:49
Second background run after cleaning in O_2 LC0043.3

Measurments in 0.2 bar of CO: (Additional note: flow here at 0.2 bar is 101 ml/min)
LC0043.0300-0399

Measurments at 0.5 bar of CO:
LC0043.0400-0499

Measurment in 1 bar of CO:
LC0043.0500-0599

LC0043.0600-0699 flush with O2

Results :

Successful measurement of both CeO_2 and KBr, the reference data provides a good fit but not perfect.

(Data saved - DRIFTS PC; Folder – Data --> L Caulfield; File name - 20230221_KBr_CeO2_modelrun)

Unique eLabID: 20230704-d890c8dedf70faf80f5920be8b43afa25134b7be
Link: https://ifgselabftw.ifg.kit.edu/experiments.php?mode=view&id=2272