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| https://upload.wikimedia.org/wikipedia/commons/thumb/3/3a/Logo_KIT.svg/800px-Logo_KIT.svg.png?20200302125831 | **LLN-ELN: Revolutionizing Experiments with Large Language Models!** | https://i.ibb.co/8XMKP9k/My-project-1.png |

# **Demo 1 for LLM in ELN**

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| No. | Question | LLM Answer | Category |
| 1 | Who is the individual or team responsible for carrying out this experiment, and what is their affiliation or role? | The individual team responsible for carrying out this experiment is Shuang Chen, and their role is a researcher at the Institute for Physical Chemistry at the Karlsruhe Institute of Technology (KIT). | Who experimented? |
| 2 | What is the room temprature to evaluate adsorption band of CO on HKUST-1? | The room temperature to evaluate the adsorption band of CO on HKUST-1 should be 30 °C. | Experimental parameters |
| 3 | What are the preparation steps for HKUST-1 in the ordered list? | Preparation steps for CO adsorption on HKUST-1 at RT  1. Put the water trap and trap containing active carbon into an oven (425 °C) overnight to remove all water and carbonyls.  2. Clean the sample chamber.  3. Load the KBr into the DRIFTS cell.  4. Check for leaks using Ar (1 atm/ 50 ml/min).  5. Test an initial background of | Procedure Stages |
| 4 | How many spectroscopy scans should be run in the CO adsorption HKUST-1 DRIFT experiment? | Eight spectroscopy scans should be run in the CO adsorption HKUST-1 DRIFT experiment. | Experimental parameters |
| 5 | What is the required heating time and temperature for the sample, and what is the cooling temperature needed afterward in HKUST-1 DRIFT experiment? | The required heating time and temperature for the sample in the HKUST-1 DRIFT experiment is 1 hour at 100°C. The cooling temperature afterwards is 30°C. | Experimental parameters |
| 6 | Where can I locate the folder for the HKUS-1 DRIFT experiment on the computer? | The folder for the HKUS-1 ‎DRIFT experiment is typically located at the D:\data\shuangchen\20230728-HKUST-1 directory on the computer. | ELN Documents Accessibility |
| 7 | What is the purpose of the experiment recorded on July 28, 2023? | he purpose of the experiment recorded on July 28, 2023 is to evaluate the adsorption bands of CO (1 atm) on HKUST-1 at room temperature (30 °C). To achieve this, the protocol involved cleaning the sample chamber, prepping the water trap and trap containing active carbon, loading KBr into the DRIFTS cell, taking background readings for KBr and HKUST-1 in Ar and CO atmospheres, running | Objective of Experiment |
| 8 | What was the primary objective or goal of the experiment conducted on July 28, 2023? | Generated Response for 2023-07-28 - CO-adsorption-on-HKUST-1-at-RT-in-drifts-28.07.2023.pdf: The primary objective or goal of the experiment conducted on July 28, 2023 was to evaluate the adsorption bands of CO (1 atm) on HKUST-1 at RT (30 °C).  Generated Response for 2023-09-01 - CO-adsorption-on-HKUST-1-at-RT-in-drifts.pdf: The primary objective or goal of the experiment conducted on July 28, 2023 was to evaluate the adsorption bands of CO (1 atm) on HKUST-1 at RT (30 °C). | Objective of Experiment |
| 9 | Can you provide detailed information about the samples utilized in the experiment, specifically HKUST-1 and KBr? | HKUST-1 is an iron-based metal-organic framework (MOF) with nanosized pores and a high surface area. It has a cubic structure composed of iron oxo (Fe3O4) and phosphonic acid (H3PO4) linkers. | Sample Description |
| 10 | Within the experiment's procedure titled "CO adsorption on HKUST-1 at RT in drifts," could you specify the temperature range and duration mentioned? | In the experiment titled "CO adsorption on HKUST-1 at RT in drifts," the temperature range is between 23°C (room temperature) and 100°C, and the duration is 1 hour. | Experimental parameters |
| 11 | In the experiment titled "CO adsorption on HKUST-1 at RT in drifts," what was the reason for heating the samples in an Ar atmosphere and subsequently cooling them down? | The reason for heating the samples in an Ar atmosphere and subsequently cooling them down is to clean them of impurities and create a more accurate and precise representation of the CO adsorption on the HKUST-1 sample when measured at RT. This process helps to remove any unwanted particles or molecules that could affect the DRIFTS measurement results. | Summary of Experiment/Conclusion |
| 12 | What were the critical parameters for performing background measurements in both Ar and CO atmospheres within the experiment "CO adsorption on HKUST-1 at RT in drifts"? | The critical parameters for performing background measurements in both Ar and CO atmospheres within the experiment "CO adsorption on HKUST-1 at RT in drifts" are:  For Ar atmosphere:  - 1 atm pressure,  - 50 ml/min flow rate,  - 256 scans,  - 2 cm-1 resolution.  For CO atmosphere:  - 1 atm pressure,  - 200 ml/min flow | Experimental parameters |
| 13 | How was the cleanliness and purity of the samples assessed during the experiment titled "CO adsorption on HKUST-1 at RT in drifts"? | The cleanliness and purity of the ‎samples were assessed during the experiment by taking a background sample in Ar atmosphere to compare the cleanliness of the samples before and after heating at 100 °C. Additionally, the water/solvent content of the sample was tested by taking a background sample in Ar atmosphere to compare the cleanliness of the sample. | Experimental Evolution |
| 14 | Could you provide additional details on the results obtained from the experiment titled "CO adsorption on HKUST-1 at RT in drifts" and any noteworthy observations made? | The results of the experiment demonstrated successful adsorption of CO on HKUST-1 at room temperature. Notable observations were observed in the spectra with the shift of strongly absorbent bands in the range of 1400-1700 cm-1. Thesubsequent flushing of the sample chamber with Ar gas for 10 minutes after the adsorption was completed resulted in the sudden drop of absorbance at the same range of wavenumbers, thus indicating successful removal of the adsorbed CO | Summary of Experiment/Conclusion |
| 15 | In what context or applications does the experiment titled "CO adsorption on HKUST-1 at RT in drifts" hold significance, and does it relate to prior research or studies? | The experiment is related to prior research as it is a common research technique which is used to investigate the adsorption of molecules on a particular material. The experiment can provide insight into the adsorption process and can be used to investigate different materials for their adsorption properties. | Usability of Experiment |
| 16 | Were there any safety precautions or considerations outlined specifically for the experiment titled "CO adsorption on HKUST-1 at RT in drifts"? | Safety precautions and considerations outlined specifically for the experiment include:  - Use of oven at 425 °C to remove all water and carbonyls  - Check for leaks using Ar (1 atm/ 50 ml/min)  - Heat the sample in Ar at 100 °C for 1 hour to clean sample  - Do not raise sample temperature above 100 °C  - Switch to CO (1 atm, 200 ml/min) and measure CO adsorption as a function of | Experiment Safety |
| 17 | What is the eLabID mentioned at the end of the document for the experiment "CO adsorption on HKUST-1 at RT in drifts," and how can I access additional information using it? | The eLabID mentioned at the end of the document for the experiment "CO ‎adsorption on HKUST-1 at RT in drifts" is 20230804-648209758ead69d055605cf8965d2bd8493d2230. You can access additional information using this eLabID by visiting the associated link, which is https://ifgselabftw.ifg.kit.edu/experiments.php?mode=view | ELN additional Information |
| 18 | What equipment and settings were used for data acquisition in the experiment? | Equipment used for data acquisition in the experiment:  DRIFTS cell; Computer; KBr powders; Ar ; CO.  Settings used for data acquisition in the experiment:  Computer settings: Folder; Spectra names;  Opus settings: Resolution 2; Phase resolution 4; Acquisition mode Double Sided, Forward-Backward; Aperture 8mm; Mode Absorbance; Detector LN MCT Narrow; Gain Automatic; ADC-counts | Equipment Setting |
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# **Demo 2 for LLM in ELN**

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| No. | Question | LLM Answer | Category |
| 1 | What were the measurement conditions for Ceria, including CO pressure levels and data ranges? | The measurement conditions for Ceria includes a CO pressure level of 2 cm-1 resolution with 512 scans and data ranges from 21 to 150°C. It was collected in a flow at room temperature before being cooled down to RT and starting batch experiments. The data was saved to the DRIFTS PC folder found in the folder "Data" and the file was named "20230411\_KBr\_References\_Temp\_Pressure\_changes." |  |
| 2 | Were there any noteworthy results or observations from the experiment involving both CeO2 and KBr? | The results of the experiment showed that the KBr data was successfully collected across a range of temperatures from 21 °C to 150 °C. Additionally, the data was saved for future use |  |
| 3 | Were there any specific challenges or issues encountered during the experiment, such as deviations from the expected results? | Yes, there were challenges and issues encountered during the experiment. One issue was that the mirrors needed adjusted, as seen in the procedure. Another issue was that in the second part of the experiment water was displacing the CO signal. The data showed that expected bands appeared, but that they were leaving the surface overtime, making it difficult to determine the results. |  |
| 4 | Could you describe the procedure followed during the experiment, including the specific steps, conditions, and any challenges encountered? | 1. Preheat CeO2 in atmosphere 225 °C overnight.  2. Perform initial background run in Ar LC0042.0.  3. Perform second background run in O2 LC0042.1.  4. Run several spectrums in O2 before heating to 750 °C.  5. Heat sample to 750 °C.  6. Close all valves, let CO run through bypass |  |
| 5 | How did the experiment address the reduction of ceria even at room temperature, and what were the implications of this observation? | The experiment addressed the reduction of ceria by heating it to two elevated temperatures and observing the results. By heating it to 50 °C and 150 °C in a CO atmosphere after cleaning it in O2, the experiment was able to detect changes in the adsorption of CO on the surface of the ceria, which is an indicator of reduction. These changes were used to gauge the extent of reduction of ceria compared to room temperature. This observation implies that the reduction of c |  |
| 6 | Were there any interesting side reactions or formations observed during the experiment, particularly involving OH groups and carbonates? | Yes, the experiment observed some interesting side reactions and formations involving OH groups and carbonates. During the 8 scan test in O2, the sample underwent an immediate reduction upon exposure to oxygen, leading to the formation of a Ce4+ with OH/coverage effect. This process was followed by a further reduction of Ce4+ ions to form Ce3+ ions, accompanied by an electron transition. Additionally, during the 0.1 bar CO dosing, the experiment observed the loss of |  |
| 7 | What were the specific details of the spectral measurements, such as the recording time, scan parameters, and recording temperature? | Recording time: 10:36 – 12:35  Scan parameters: 8 scans with Ar atmosphere, 8 scans with O2, 256 scans with O2, 512 scans with 0.1 bar, 256 scans with Ar  Recording temperature: 753°C (heat to 1000°C, keep 2 hours), 1000°C (776°C), 30°C (after heating) in O2. |  |
| 8 | Can you elaborate on the reasons for conducting transient DRIFTS measurements after exposure to CO and switching to Ar, and what insights were gained from this transition? | Transient DRIFTS measurements were conducted after exposure to CO and switching to Ar in order to gain insight into the oxidation state of the ceria sample and to observe the surface redox and coverage effects of oxidation and reduction. The DRIFTS measurements detect the presence of absorbed molecules into the material and provide spectral information to help clarify the oxidation states of the samples. By switching from CO to Ar, it is possible to observe the changes in surface chemistry that take place upon oxidation/reduction |  |
| 9 | What motivated the decision to measure bands at ~2175 cm-1and 2168 cm-1, and how did these specific bands relate to the experiment's goals? | The decision to measure bands at ~2175 cm-1and 2168 cm-1 was based on the goal of the experiment to investigate polycrystalline ceria at high pressures and high temperature after cleaning with O2. These specific bands related to the experiment's goals because they were used to identify changes in the ceria sample due to the oxygen and pressure treatments. The 2175 cm-1 band was used to characterize ceria with Ce3+ ions, while the 2168 |  |
| 10 | What was the purpose of conducting background runs in both Ar and O2, and how did these runs contribute to the experiment? | The purpose of conducting background runs in both Ar and O2 was to create a reference spectrum that could be compared to the spectra generated at different pressures of CO in order to observe the effect of the pressure changes on the adsorption bands. These reference spectra allowed for the removal of the gas-phase signal, which could interfere in the interpretation of the results. Therefore, these background runs were important for the success of the experiment. |  |