Installing the project

1. Download python
    a. Directly download it via …
    b. Use a dedicated environment using conda (or anaconda etc, see their documentation on how to install the packages)
2. Run */setup.py* to install the required packages
    a. Alternatively, you can use pip in the command prompt/terminal *pip install -r ./requirements.txt*

Configuring SQLite databases

3. Download the following from the HITRAN database and order the files following the example of Table 1;
    a) line-by-line datasets from https://hitran.org/lbl/
        i. need the .par file
        ii. rename file as "dd_HITRAN_data.par", where "dd" are two digits of the molecule ID (e.g. 02, 11, ..)
    b) molparam.txt https://hitran.org/docs/iso-meta/
    c) partition sum lists for all isotopologues of the molecule from https://hitran.org/docs/iso-meta/

Table 1: An example for CH4 on how to install the files downloaded from HITRAN.

/ch4	*/raw*	*/06_HITRAN_dat.par*
/ch4	*/raw*	*/molparam.txt*
/ch4	*/q32.txt*	
/ch4	*/q33.txt*	
/ch4	*/q34.txt*	
/ch4	*/q35.txt*	

4. Run the respective python script found under */ftir_data_processing/generate_database* *to obtain the sqlite database similar to shown in* Table 2.

Table 2: Output generating sqlite database.

/ch4	*/raw*	*/parsum.dat*
/ch4_database.sqlite		

Test the code

5. Simulate IR absorption spectra using the scripts found in /ftir_data_processing/simulate_specra/

If it can simulate the spectra, then I can fit your measured spectra