Short discussion of the theory behind your project, and about code presentation and illustration of results. Also feel free to discuss difficulties and how you have addressed them.

The theory behind this project was that this method is based on the orthogonal scheme to directly solve the H-matrix. Furthermore, the H-matrix setup was similar to extended Huckel theory in homework 3 except, in this paper they zeroed out the off-diagonals with parameters that they studied were most helpful to calculate the off-diagonals such as beta, lambda, bohr radius and internuclear distance. Similarly, the paper directly solved for the eigenvalues from the H-matrix to calculate the total energy in addition to an extra step, which was the nuclear energy.

The difficulties I have experienced were the creation of the H-matrix because there are multiple orbitals that belong to the carbon atoms, but I could not find a way to properly filter the carbon-hydrogen and carbon-carbon bonds that would apply the proper parameters depending on which carbon orbitals were interacting with the other atomic orbitals. It seems that the mechanism I chose to filter the parameters by the atomic bonds that were H-H, C-H, and C-C. Then I would use atomic numbers and angular momentum (l) to separate out the different possibilities of C-H bond pairs that were possible ss or sp-pairs. Lastly, the C-C pair would lead to pp-pairs. Thus, when the molecules include carbon and become larger, the H-matrix would not be set up properly to solve for the right eigenvalues.

The only result I was able to get from writing my code for MTB/2 method was diatomic hydrogen gas that was 0.104 kcal/mol versus the calculated 0.0 kcal/mol that was shown in the paper. I also used different coordinates provided from class that are in atomic units instead of the NIST angstrom coordinates that resulted in a slightly different calculation of 0.16kcal/mol in the h2 directory.

In conclusion, I would like to overcome these coding difficulties by changing the data structure and making sure what type of data I have access to. I noticed that the 47 molecules in table 2 I was supposed to find the heat of formation for had a lot of missing cartesian coordinate data as the molecules got larger. I am not sure how the paper was able to obtain this information. Furthermore, I decided this is where I would stop my project due to limited information . Additionally, I would change my code by inputting internuclear distances that are found but it was too difficult to implement such a huge change to my already written code based on the cartesian coordinates that I later found out were mostly unavailable. Also, I may reimplement my code by mapping instead of filtering by conditions of the atomic orbital pairs. I found this to be an issue in CDNO2 because some of the condition statements were faulty. Furthermore, my code is written to only take an even number of electrons that scale directly to the dimensions of the matrix. I could not find the total energy of the organic molecules online. I could only find the heat of combustion, for instance, ethane.