UNIVERSITY OF CALIFORNIA BERKELEY

Numerical Algorithms Applied to Computational Quantum Chemistry
Grading Rubric for Homework 5

5.1 **Derivation** Derive the correct forms of $x_{\mu\nu}$ and y_{AB} for the analytical gradient of CNDO/2 energy. You must upload a PDF document that details your derivation process on Gradescope. This will be due by the first monday. A solution will be released immediately afterwards.

i. **Derivation of $x_{\mu\nu}$ (2 points):**

ii. **Derivation of y_{AB} (2 points):**

iii. **Derivation of Derivatives for Overlap Integrals (1 point):**

5.2 **Implementation** You are required to calculate and print the the following derivatives with respect to atomic coordinates. Ensure these are printed in your output.

i. **Overlap Integrals $S_{\mu\nu}^{\mathbf{R}_A}$ (2 points):**

ii. **Two-Electron Integrals $\gamma_{AB}^{\mathbf{R}_A}$ (2 points):**

iii. **Nuclear Repulsion Energy $V_{\text{nuc}}^{\mathbf{R}_A}$ (1 points):**

iv. **Compute the total gradient of CNDO/2 energy (2 points):**

Bonus: **Geometry Optimization (1 point):** Experiment with your CNDO/2 gradient in conjunction with an optimization method from HW1 to optimize structures of molecules (such as N_2 and O_2). Share any interesting insights or findings from your optimization. For reference structures of common molecules, you can go to CCCBDB `https://cccbdb.nist.gov/expgeom1x.asp`.