

Course Title

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Due Date

1 Problem

1.a Part A

$h_{A_t O_t}^{A_f O_f} \rightarrow A_f = \text{Atom From } A_t = \text{Atom to}$
 $O_f = \text{Orbital From } O_t = \text{Orbital To}$

$$H = \begin{pmatrix} h_{1,1}^{1,1} & h_{1,2}^{1,1} & h_{1,3}^{1,1} & \cdots & h_{2,1}^{1,1} & h_{2,2}^{1,1} & \cdots \\ h_{1,1}^{1,2} & h_{1,2}^{1,2} & h_{1,3}^{1,2} & \cdots & h_{2,1}^{1,2} & h_{2,2}^{1,2} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\ h_{1,1}^{1,11} & h_{1,2}^{1,11} & \cdots & & \ddots & & \\ h_{1,1}^{2,1} & h_{1,2}^{2,1} & \cdots & & & \ddots & \\ \vdots & \vdots & \vdots & & & & \end{pmatrix}$$