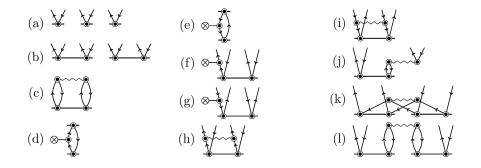
CHEM-8950 Quiz 4 April 20th, 2020

Question 1. For each of the following expectation values:

- i Write down the diagrammatic representation (Do not form contractions)
- ii Does the term contribute to the pentuples amplitudes in CCSDTQP? Explain why or why not in terms of excitation levels and/or connected/disconnected terms

$$\langle \Phi^{abcde}_{ijklm} | H_c T_2 T_4 | \Phi \rangle$$
$$\langle \Phi^{abcde}_{ijklm} | H_c T_3 | \Phi \rangle$$
$$\langle \Phi^{abcde}_{ijklm} | H_c T_2 T_3 T_4 | \Phi \rangle$$

Question 2. Translate the following diagrams into algebraic expressions and show your work



Question 3. Evaluate the following expectation values using diagrams and show your work. Be sure to translate the resulting diagrams back into algebraic expressions:

$$\begin{split} \langle \Phi | C_1^{\dagger} H_c C_1 \Phi \rangle \\ \langle \Phi | H_c (1 + T_2 + \frac{1}{2} T_2^2) | \Phi \rangle \\ \langle \Phi_{ij}^{ab} | H_c (\frac{1}{2} T_2^2) \Phi \rangle \end{split}$$

Use
$$C_1 = c_a^i \tilde{a}_i^a$$
, $T_2 = (\frac{1}{2!})^2 t_{ab}^{ij} \tilde{a}_{ij}^{ab}$