A First Course on Kinetics and Reaction Engineering

How To Calculate a Heat of Reaction*

1. Determine the stoichiometric coefficient, including sign, of every species that participates in the reaction.
2. Find values for the standard heat of formation at 298 K for every species that participates in the reaction, or find values for the standard heat of combustion at 298 K for every species that participates in the reaction.
   a. Note that the heat of formation of elements will usually equal zero and heats of combustion for the standard combustion products (CO_2, $H_2O_{(l)}$, etc.) will usually equal zero or simply won't be included in the table.
3. When finding the standard heats of formation or combustion in step 2, take note of the standard states used for all species (that is those that participate in the reaction being analyzed as well as either the elements appearing in the formation reactions or the combustion products appearing in the combustion reactions).
4. Calculate the standard heat of reaction at 298 K using the data from steps 1 and 2 using equation (2.1) from the informational reading if heats of formation were found in step 2 or equation (2.2) if heats of combustion were found in step 2. This is the heat of reaction at 298 K when all the species are in their standard states.
5. For each species participating in the reaction being analyzed, determine whether it will undergo a phase change upon heating/cooling from 298 K to the desired temperature for the heat of reaction (i. e. is its phase in the reaction being analyzed different from its phase in the standard formation or combustion reactions?).
   a. If a phase change will occur
      i. Find the heat capacity for the species in its standard state and integrate that heat capacity from 298 K to the phase change temperature
      ii. Find the latent heat for the phase change at the phase change temperature
      iii. Find the heat capacity for the species in the new phase and integrate that heat capacity from the phase change temperature to the desired temperature for the heat of reaction
      iv. Add the heats from the three preceding steps together, multiply by the stoichiometric coefficient of the species in the reaction being analyzed, and add the result to the heat of reaction from step 4
   b. If no phase change will occur, find the heat capacity for the species in its standard state and integrate that heat capacity from 298 K to the desired temperature for the heat of reaction, multiply the result by the stoichiometric coefficient of the species in the reaction being analyzed, and add the result to the heat of reaction from step 4

* Every reaction is unique, but in very many cases the standard heat of a reaction can be calculated by following the steps given here.