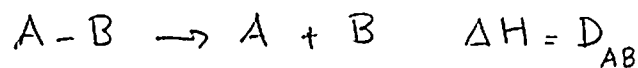


Estimating $\Delta H_{\text{reaction}}$ from bond energies

"Bond energy" is defined to be "bond dissociation energy"

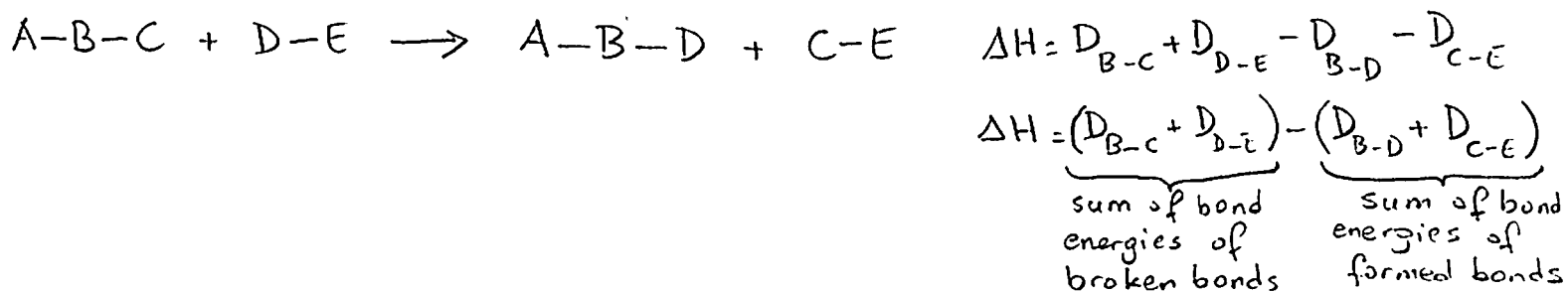
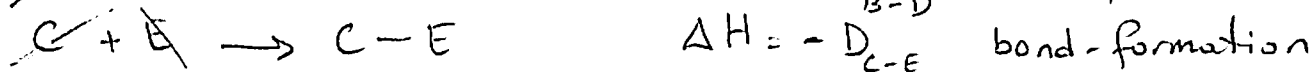
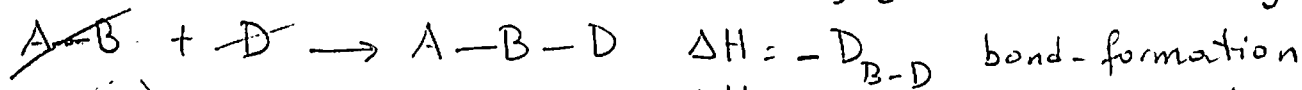
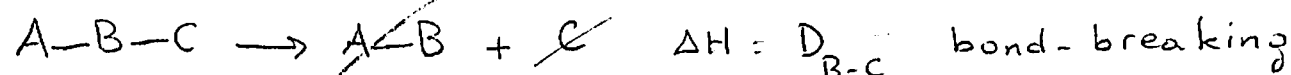


In a reaction, one or more of the bonds in the reactants are broken, and one or more newly formed bonds appear in the products.

We can break down the reaction into individual bond-breaking and bond-making steps:



can be broken down into:



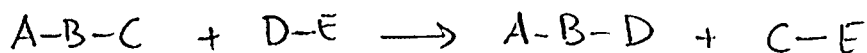
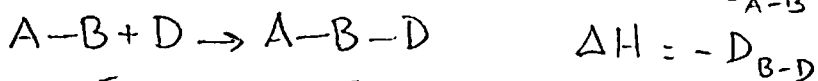
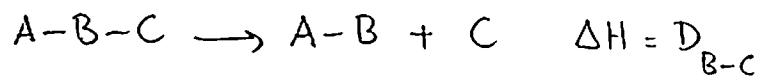
We can generalize this to any reaction:

$$\Delta H_{\text{reaction}} = \left(\text{Sum of bond energies} \right)_{\text{broken}} - \left(\text{Sum of bond energies} \right)_{\text{formed}}$$

If you find it difficult to find all the broken and formed bonds, you can pretend that all of the bonds in the reactants are broken, and then all the bonds in the products are newly formed. While this involves adding up more numbers, it may be more foolproof because it involves mechanically counting every bond rather than discerning which bonds are broken (no longer seen in products) and which bonds are newly formed (seen in products but not in the reactants). Bonds that remain intact cancel out in the end. In this formulation, we have:

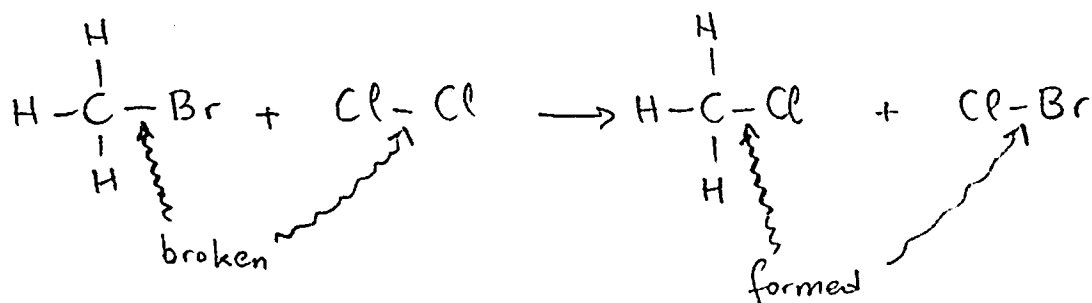
$$\Delta H_{\text{reaction}} = (\text{Sum of all bond energies})_{\text{reactants}} - (\text{Sum of all bond energies})_{\text{products}}$$

It corresponds to the following steps for the previous example:



$$\Delta H = \overbrace{(D_{B-C} + D_{A-B} + D_{D-E})}^{\text{bond energy of reactants}} - \underbrace{(D_{A-B} + D_{B-D} + D_{C-E})}_{\text{bond energy of products}}$$

Example:



$$\Delta H = (D_{\text{C-Br}} + D_{\text{Cl-Cl}}) - (D_{\text{C-Cl}} + D_{\text{Cl-Br}})$$

or we can use the second method and sum up over all the bonds in reactants and products, whether they stay intact or not

$$\Delta H = (3D_{\text{C-H}} + D_{\text{C-Br}} + D_{\text{Cl-Cl}}) - (3D_{\text{C-H}} + D_{\text{C-Cl}} + D_{\text{Cl-Br}})$$