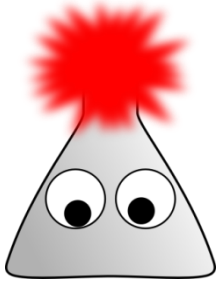
Visualizing the Energy of Chemical Reactions

Reaction Coordinate Diagrams



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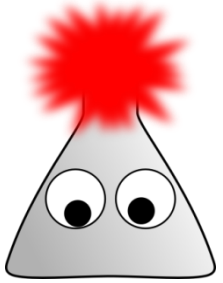
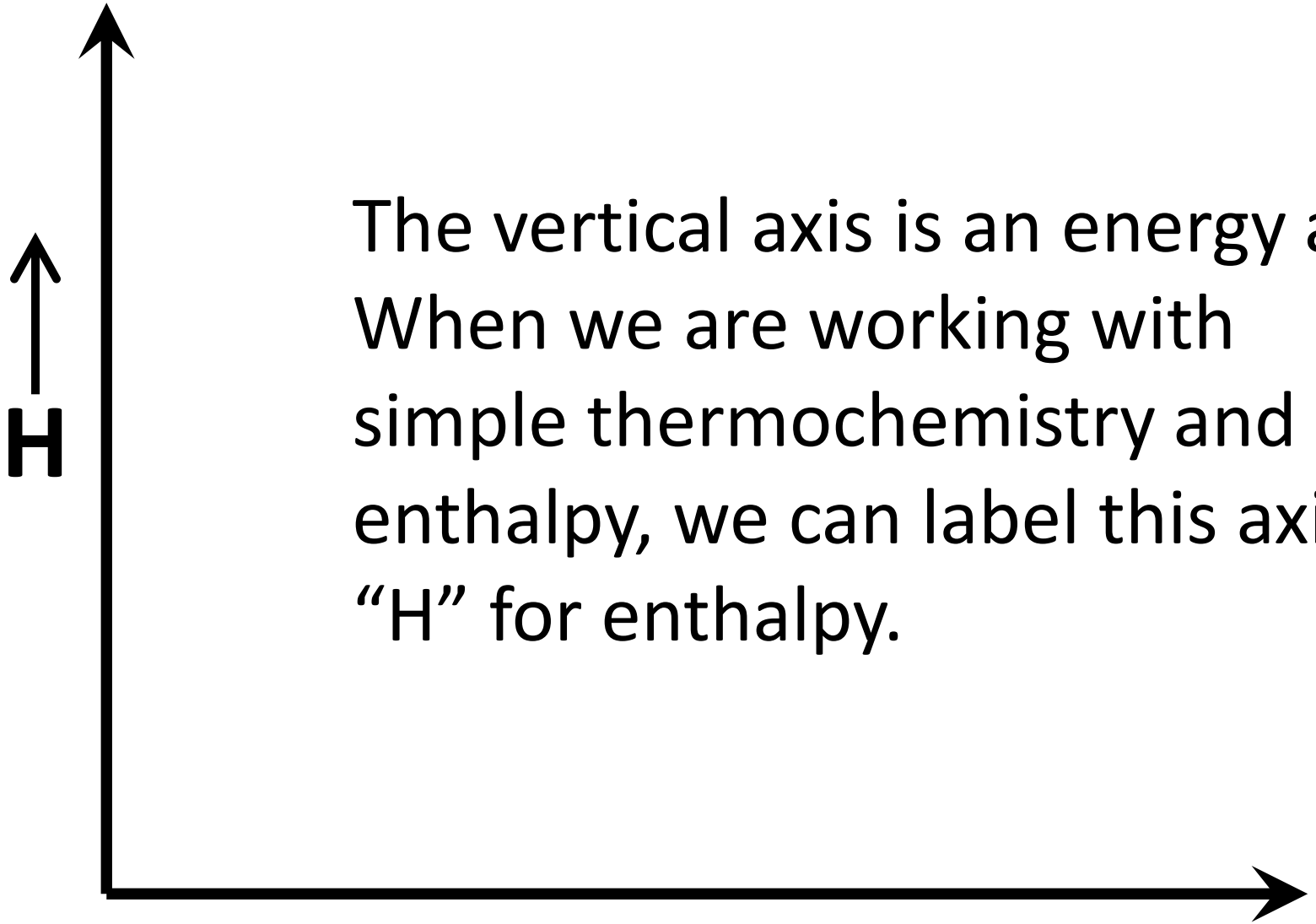
There are a number of ways to visualize chemical reactions with varying degrees of complexity.

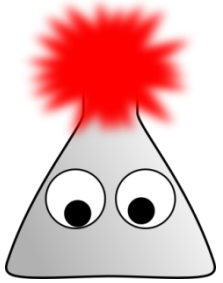
One way to visualize chemical reactions that is very information-rich while not being overly abstract is by use of a reaction coordinate diagram. Reaction coordinate diagrams allow us to follow the energy of a system as it undergoes various physical and chemical transformations.



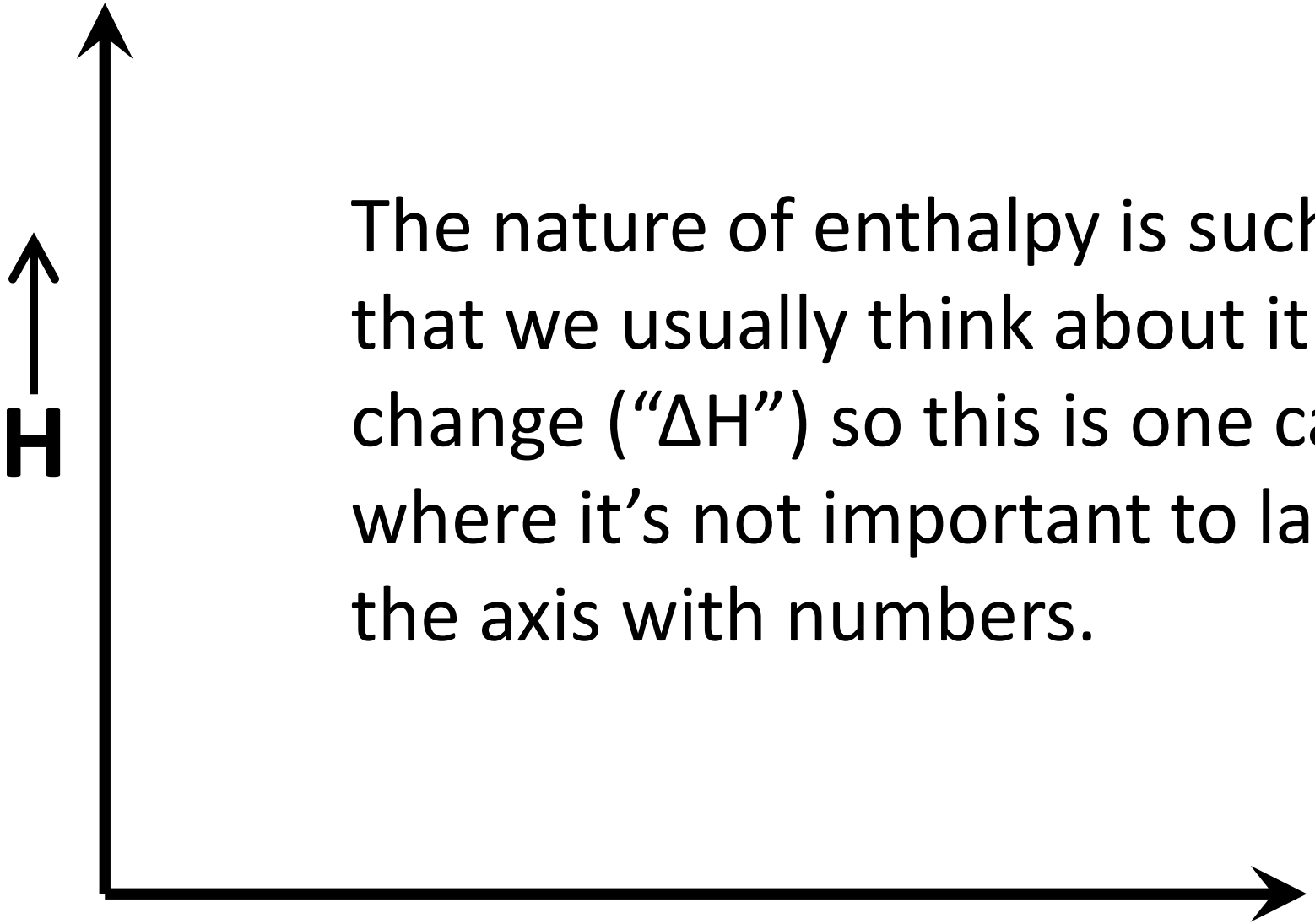
Rxn Coordinate Diagrams



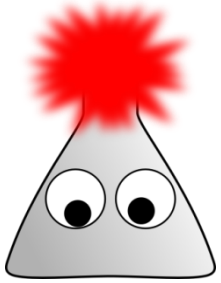
The vertical axis is an energy axis. When we are working with simple thermochemistry and enthalpy, we can label this axis "H" for enthalpy.



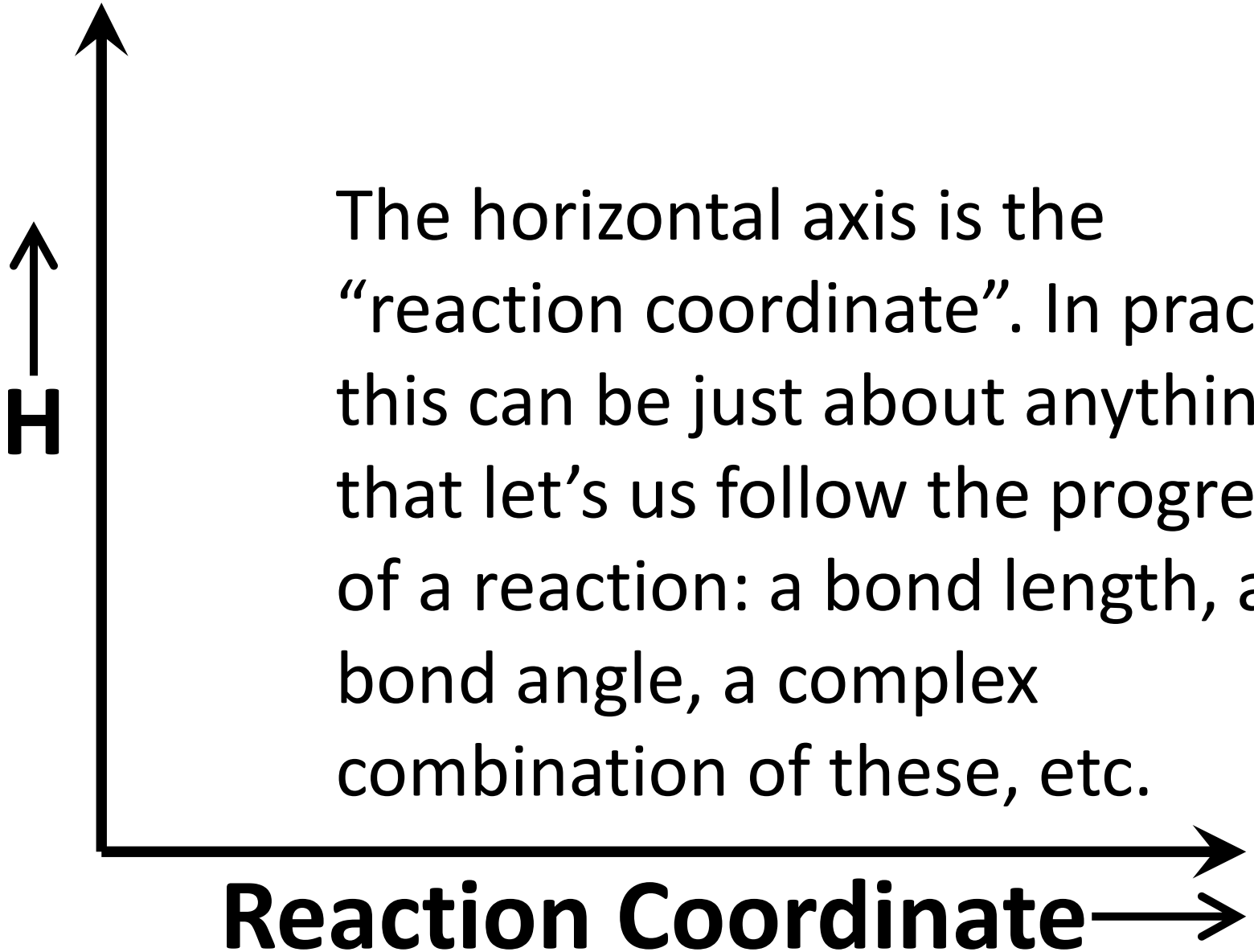
Rxn Coordinate Diagrams



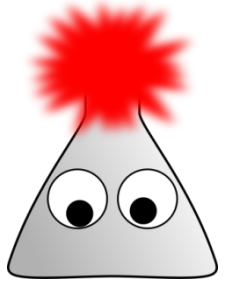
The nature of enthalpy is such that we usually think about it as a change ("ΔH") so this is one case where it's not important to label the axis with numbers.



Rxn Coordinate Diagrams



The horizontal axis is the "reaction coordinate". In practice, this can be just about anything that let's us follow the progress of a reaction: a bond length, a bond angle, a complex combination of these, etc.



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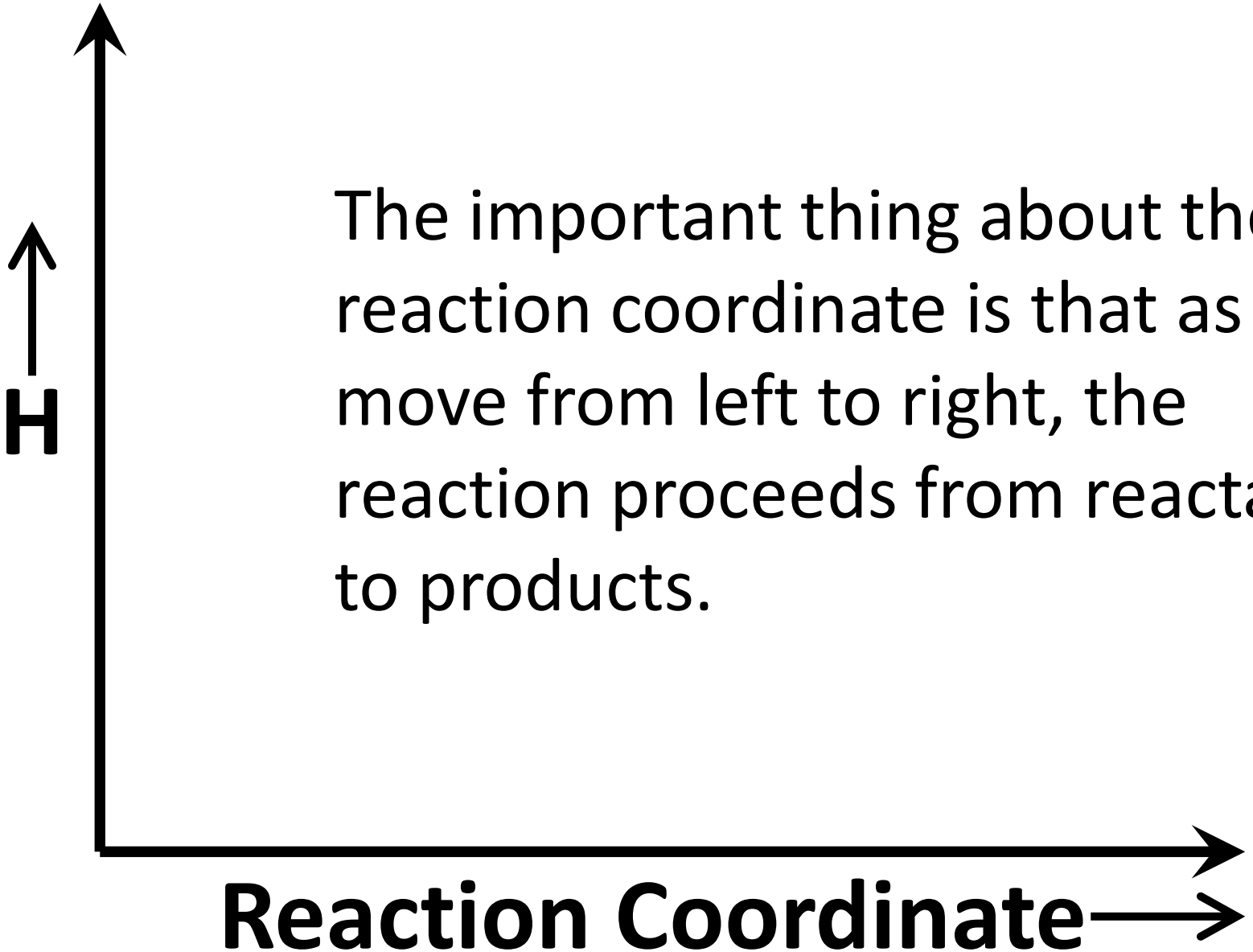
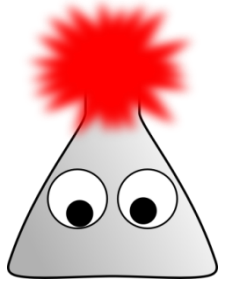
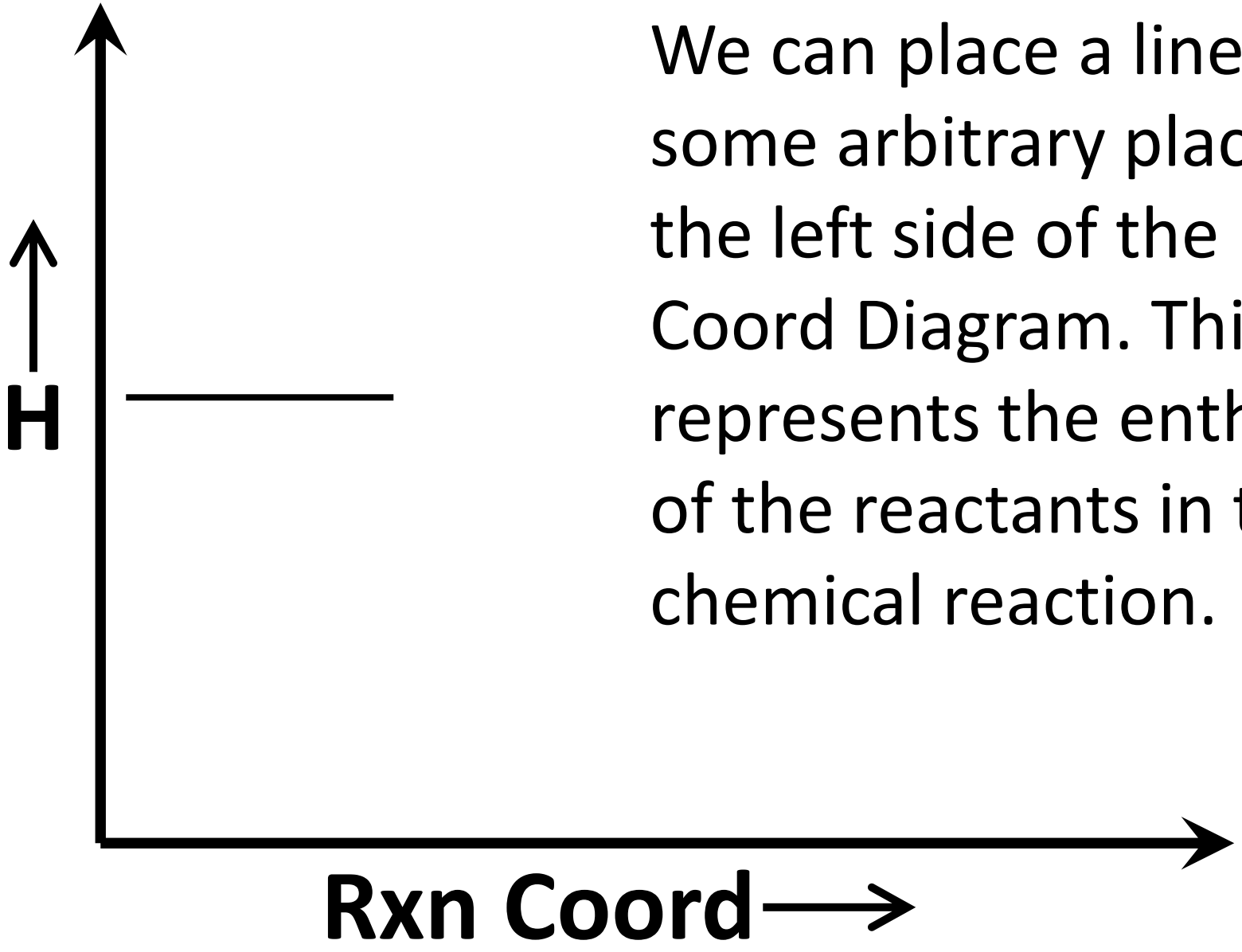
Rxn Coordinate Diagrams



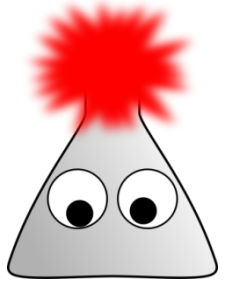
The important thing about the reaction coordinate is that as we move from left to right, the reaction proceeds from reactants to products.



Rxn Coordinate Diagrams



We can place a line at some arbitrary place on the left side of the Rxn Coord Diagram. This represents the enthalpy of the reactants in the chemical reaction.



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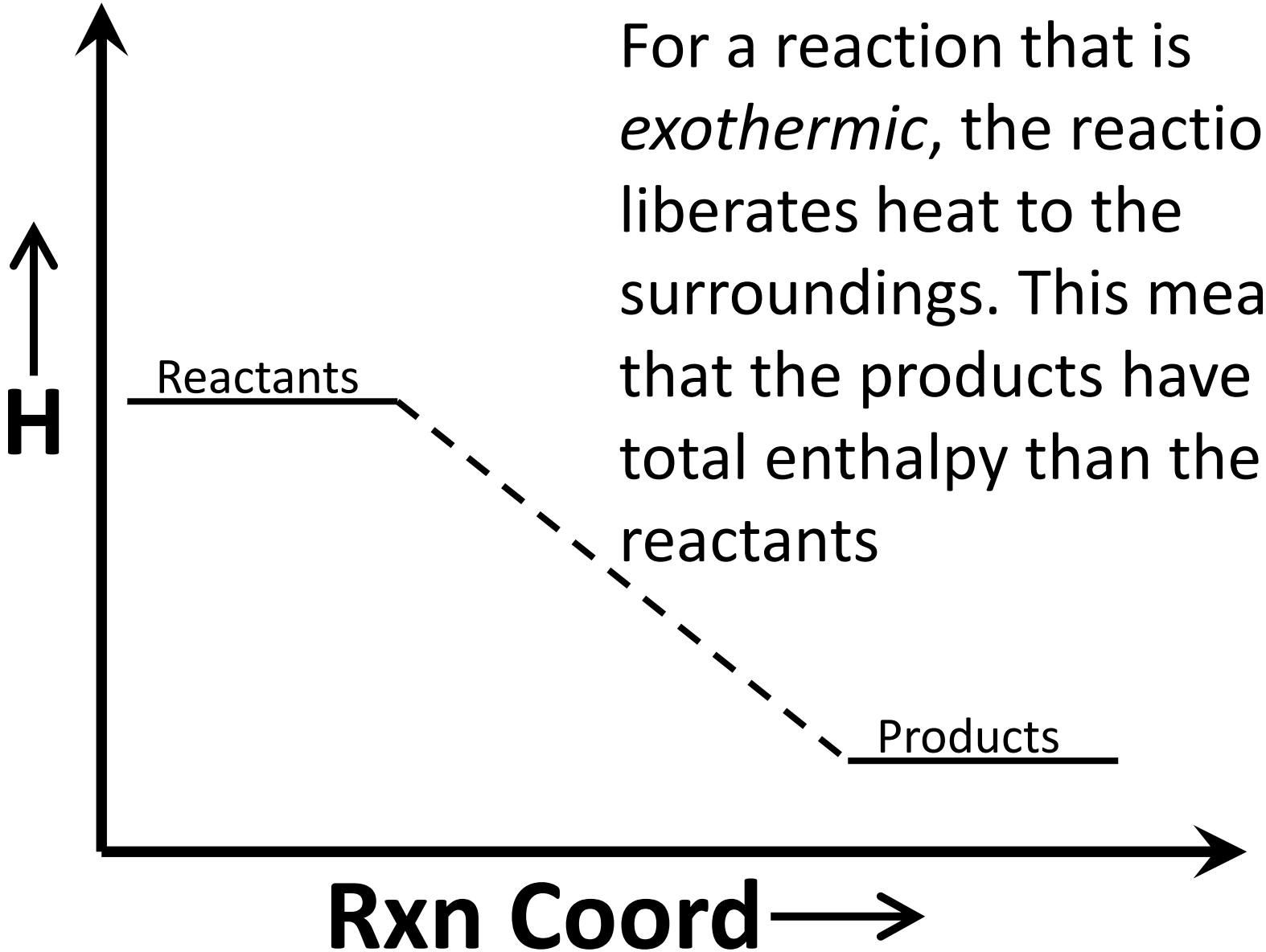
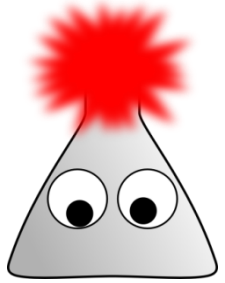


For a reaction that is *exothermic*, the reaction liberates heat to the surroundings. This means that the products have *less* total enthalpy than the reactants



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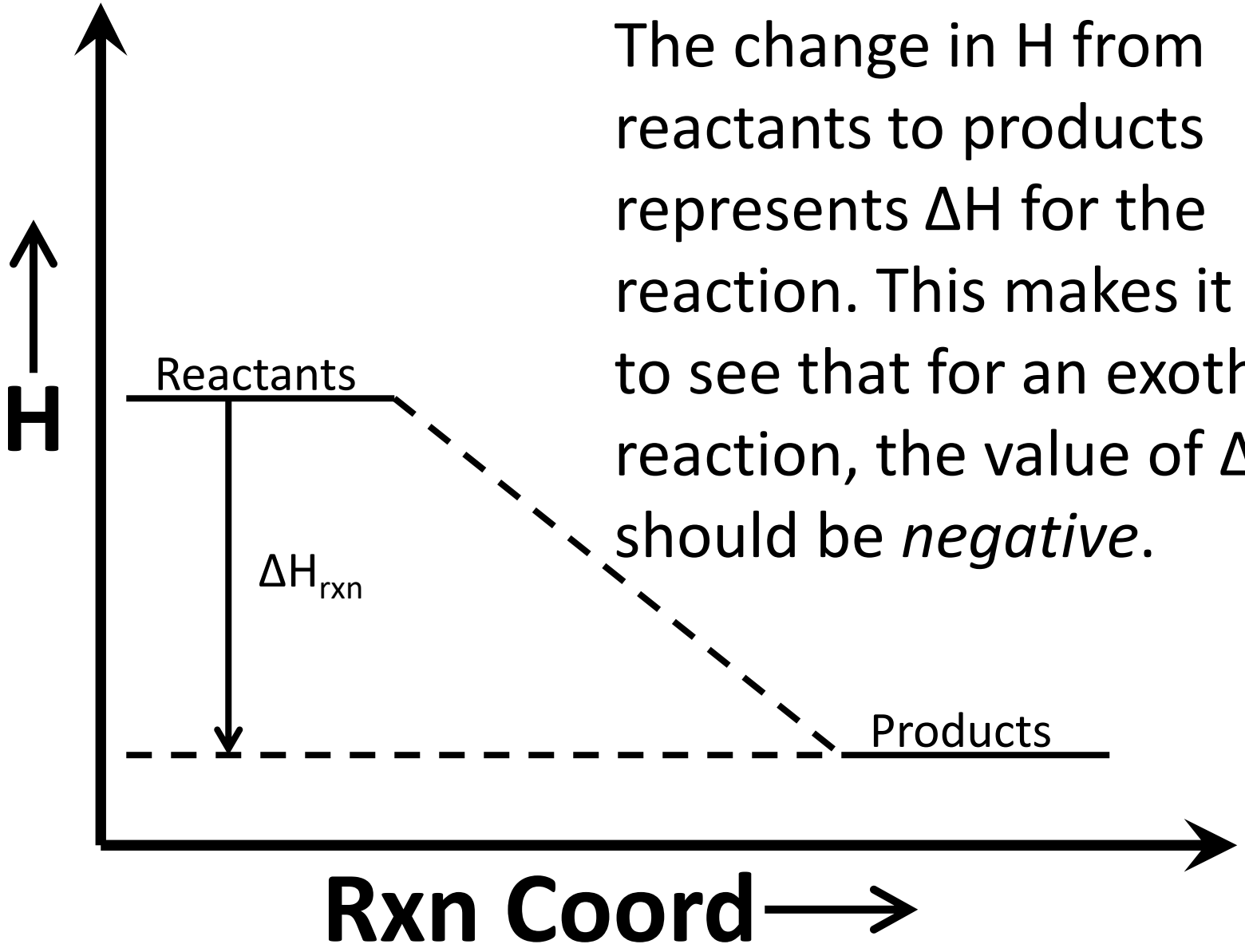
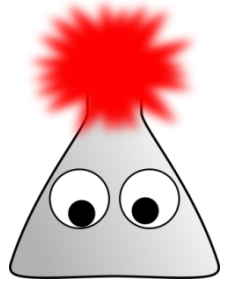
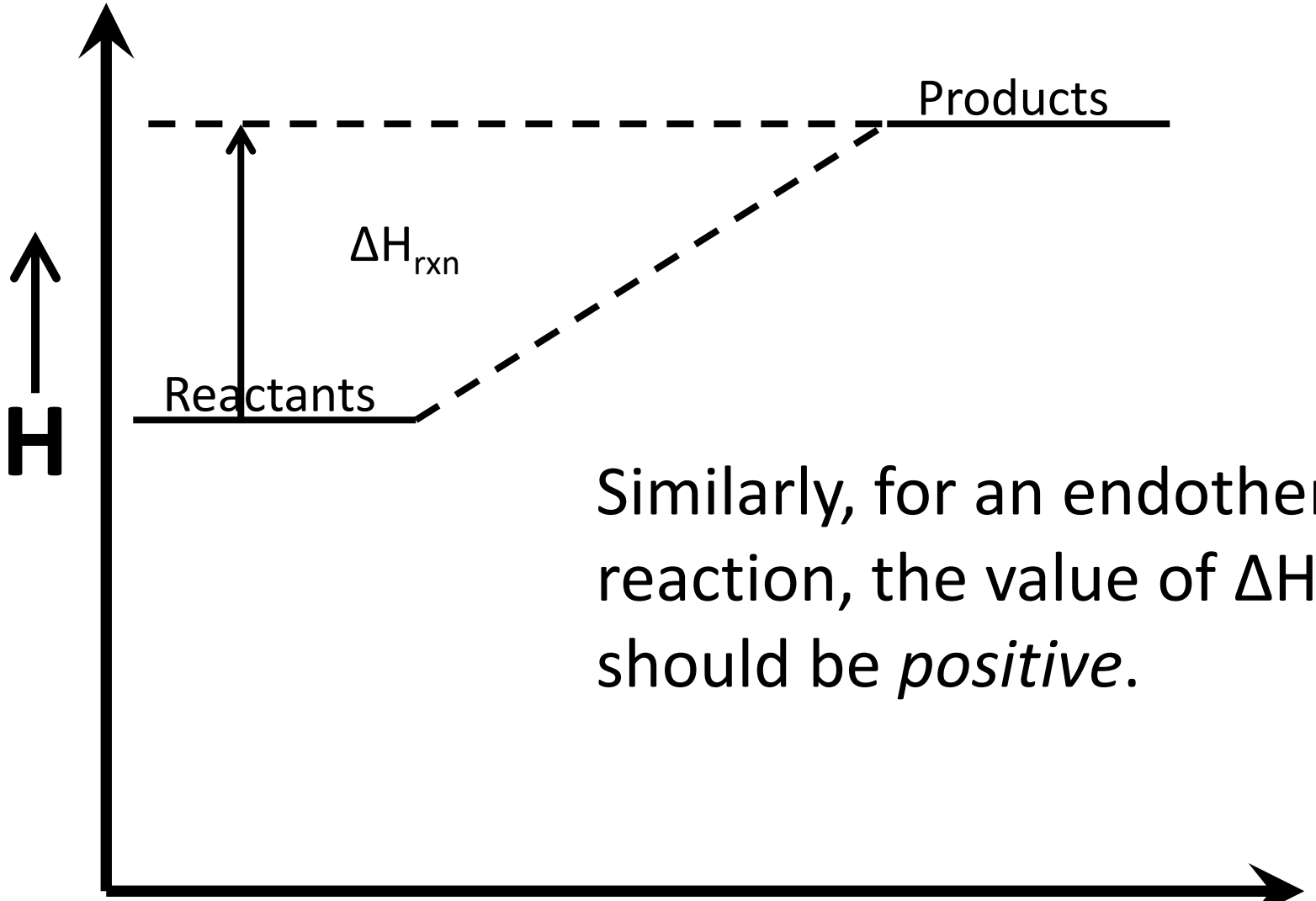


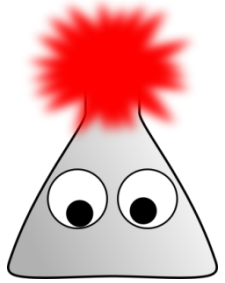
The change in H from reactants to products represents ΔH for the reaction. This makes it easy to see that for an exothermic reaction, the value of ΔH_{rxn} should be *negative*.



Rxn Coordinate Diagrams



Similarly, for an endothermic reaction, the value of ΔH_{rxn} should be *positive*.



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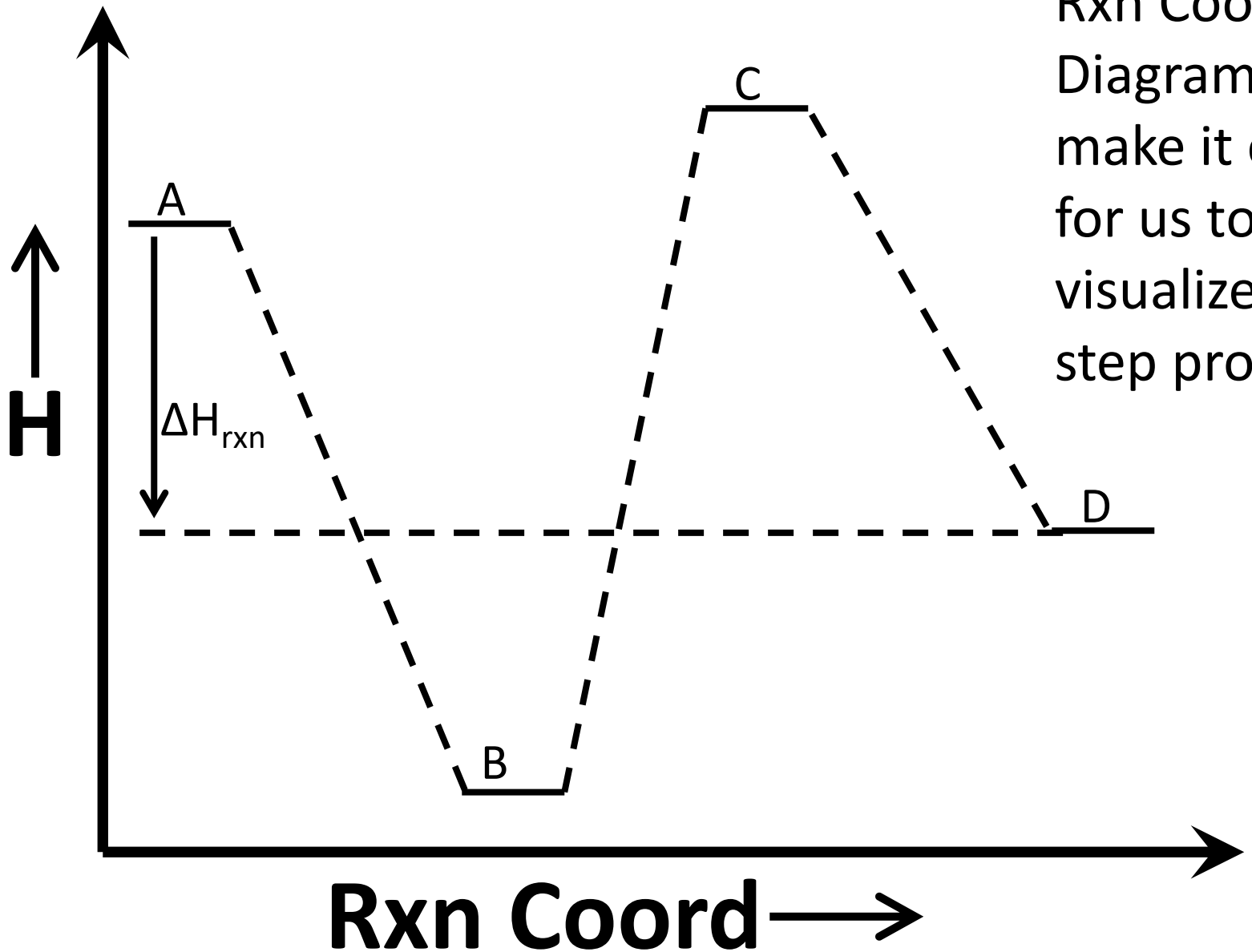
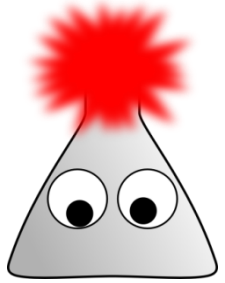


Rxn Coord Diagrams also make it easier for us to visualize multi-step processes



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