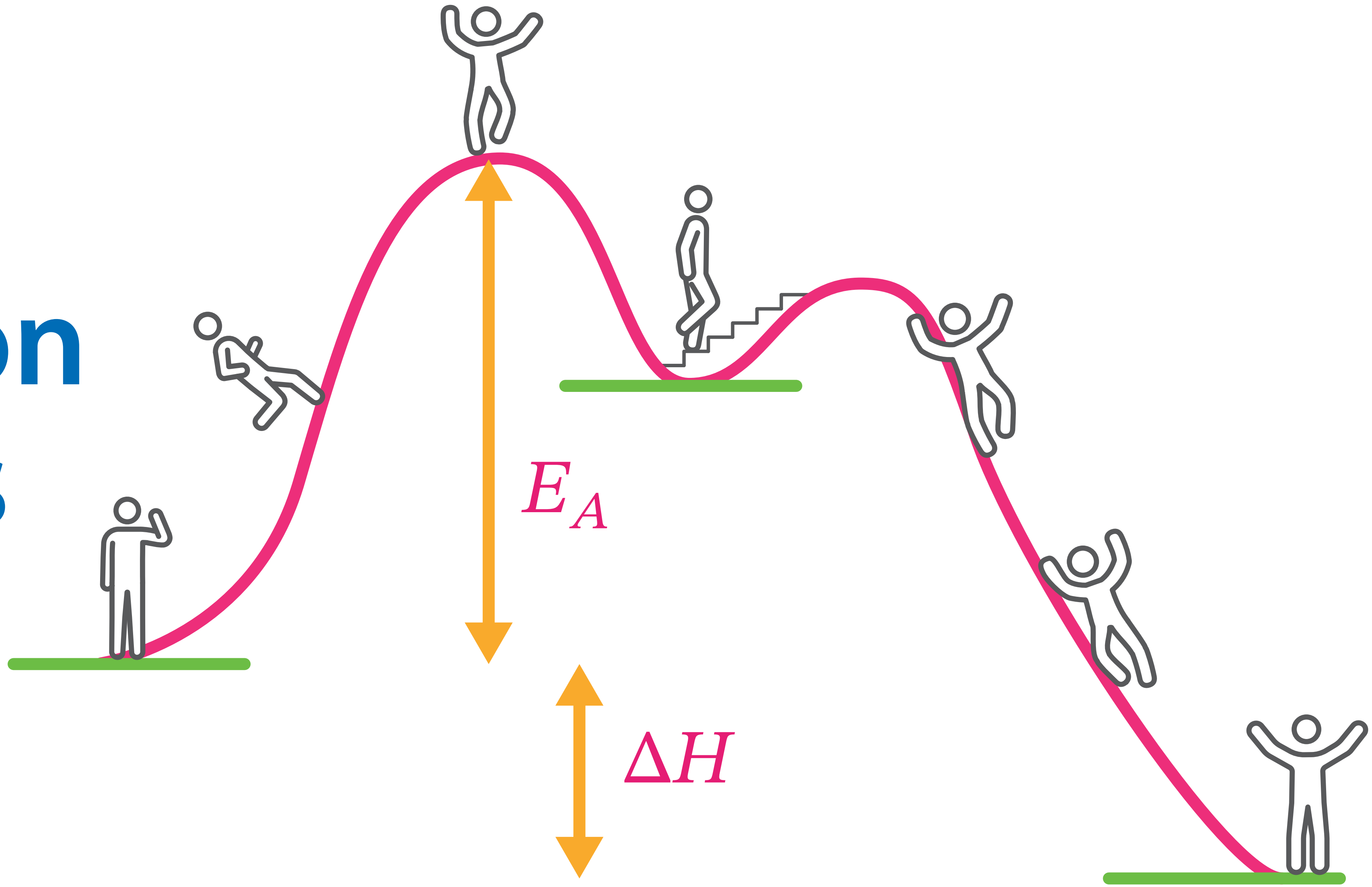
Reaction Profiles



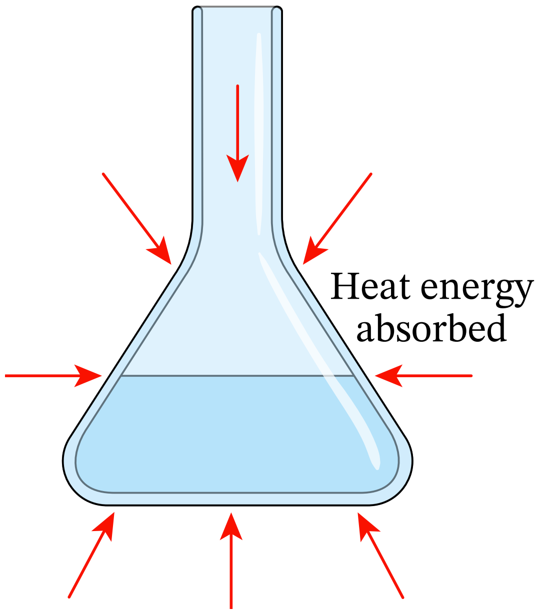
Lesson Objectives

You will be able to

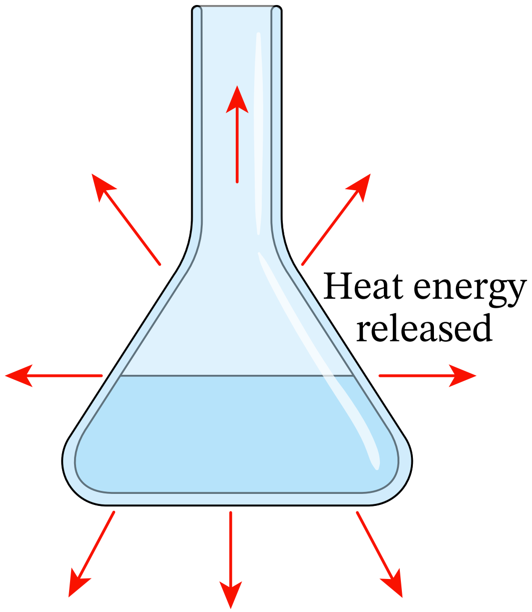
- understand a reaction profile,
- identify where the products, reactants, transition states, and energetic barriers are on a reaction profile,
- correctly label a reaction profile diagram with the energy changes ΔH, and E_a,
- identify whether a reaction is exothermic or endothermic based on a reaction profile.

Chemical Reactions and Energy Changes

Whenever a chemical reaction occurs, there are accompanying energy changes.



As a result, reactants and products can have a different amount of energy from each other.

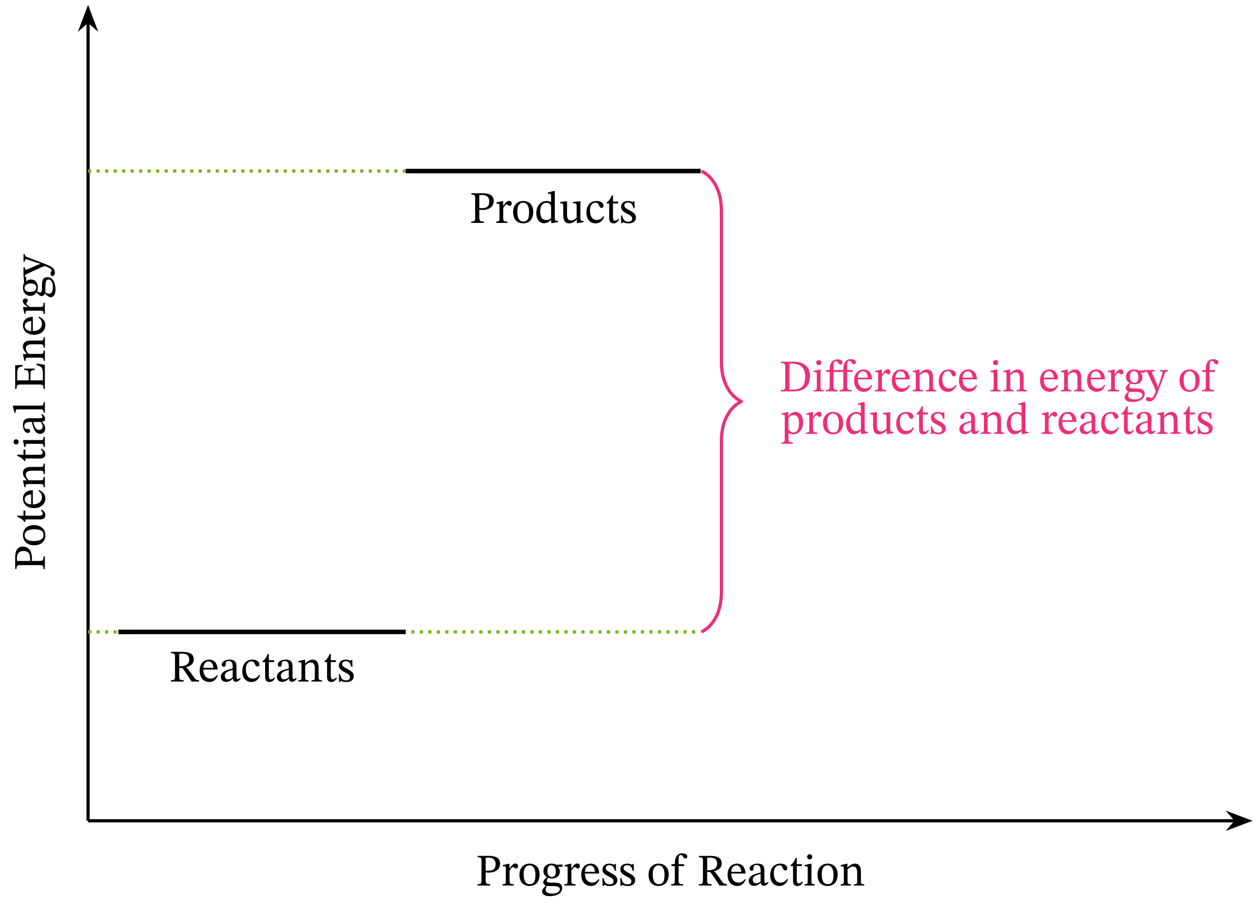


Energy Level Diagram

Chemists can use very simple energy level diagrams to show how the total potential energy changes as reactants turn into products during a chemical reaction.

The *y*-axis of an energy level diagram represents the potential energy of the substance, which is a summation of the different energies stored in the chemical substance.

It can be expressed with numbers and units such as kilojoules per mole (kJ/mol). However, it is sometimes appropriate to show energy level diagrams without any units whatsoever.



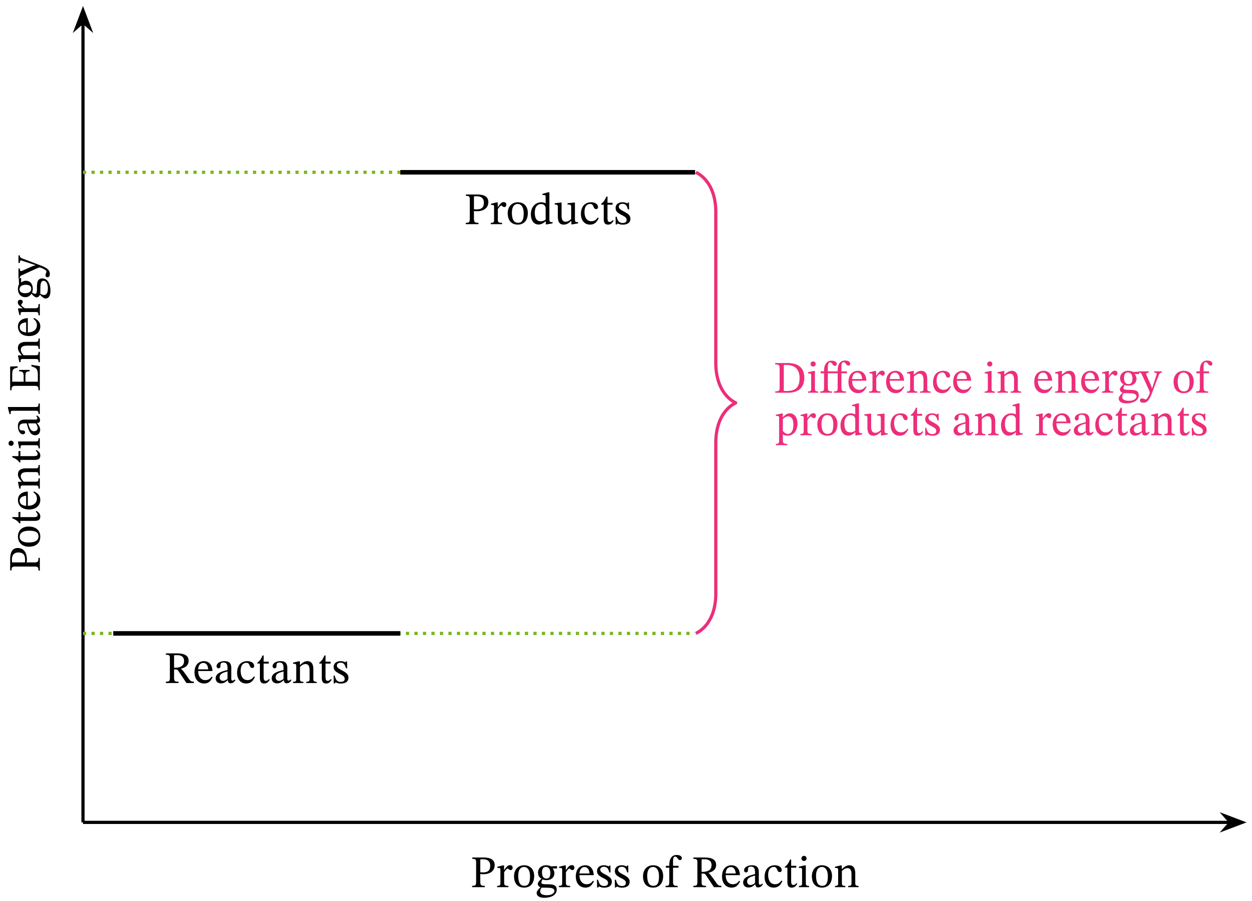
Energy Level Diagram (Continued)

The x-axis represents the reaction coordinate, or the progression of the reaction from reactants to products.

Units are not usually used for the x-axis, because it does not represent time or any other familiar physical quantity.

The difference in the energy between the products and the reactants is called the enthalpy change and is given the symbol ΔH:

$$\Delta H = \text{energy of products} - \text{energy of reactants.}$$



Definition: Enthalpy Change (ΔH)

Enthalpy change is the difference in energy between the products and the reactants.

Relation between Potential Energy and Stability

As the potential energy of any molecule increases, its stability decreases, meaning it becomes more reactive.

On the other hand, a decrease in the potential energy of any molecule, means its stability increases, and it becomes less reactive.

Thus, the molecule stability and its potential energy are inversely proportional to each other.

Endothermic Reactions

Endothermic chemical reactions absorb heat energy, and they usually cause the surrounding temperature to decrease either slightly or significantly.

In any endothermic chemical reaction, the potential energy of the product molecules is always higher than the potential energy of the reactant molecules.

The products are less stable and more reactive than the reactants.

The enthalpy of the products is greater than the enthalpy of the reactants, and thus the change in enthalpy (ΔH) is positive.

Energy Level Diagram for Endothermic Reactions

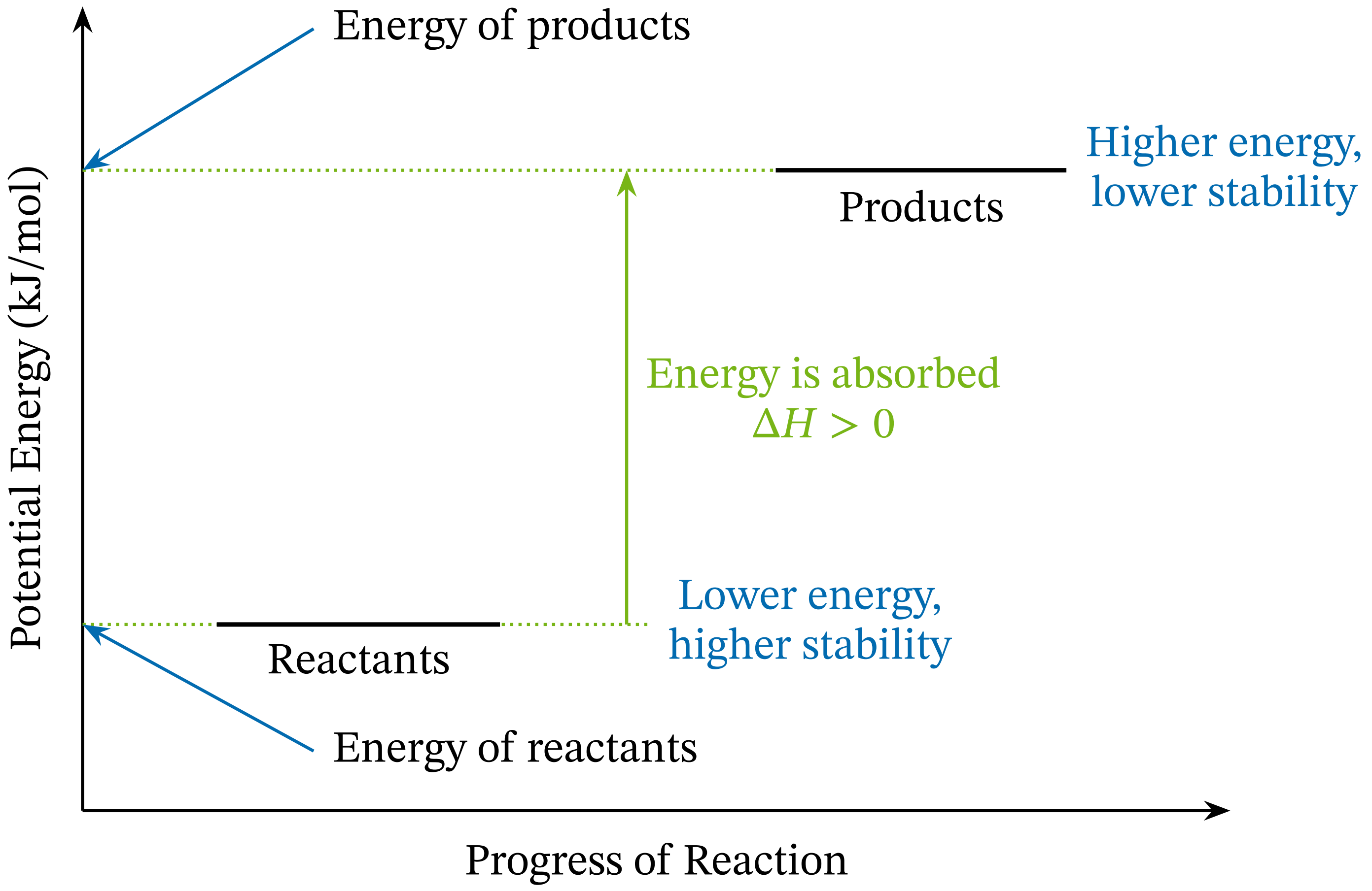
The opposite energy level diagram shows the potential energy of the reactants and the products during a simple endothermic reaction.

The diagram shows that the system absorbs heat energy as the reaction occurs.

The energy absorption process is represented by the green arrow that stretches from the reactants line to the products line.

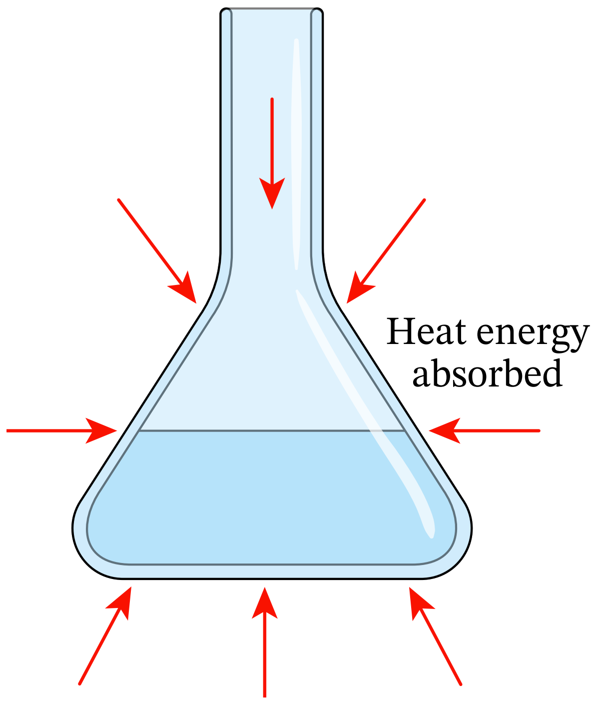
The difference in the energy between the products and the reactants is called the enthalpy change and is given the symbol ΔH:

$\Delta H =$ energy of products − energy of reactants.



Definition of Endothermic Reactions

An endothermic reaction is a chemical reaction where energy is absorbed by the reacting chemicals from the surroundings.



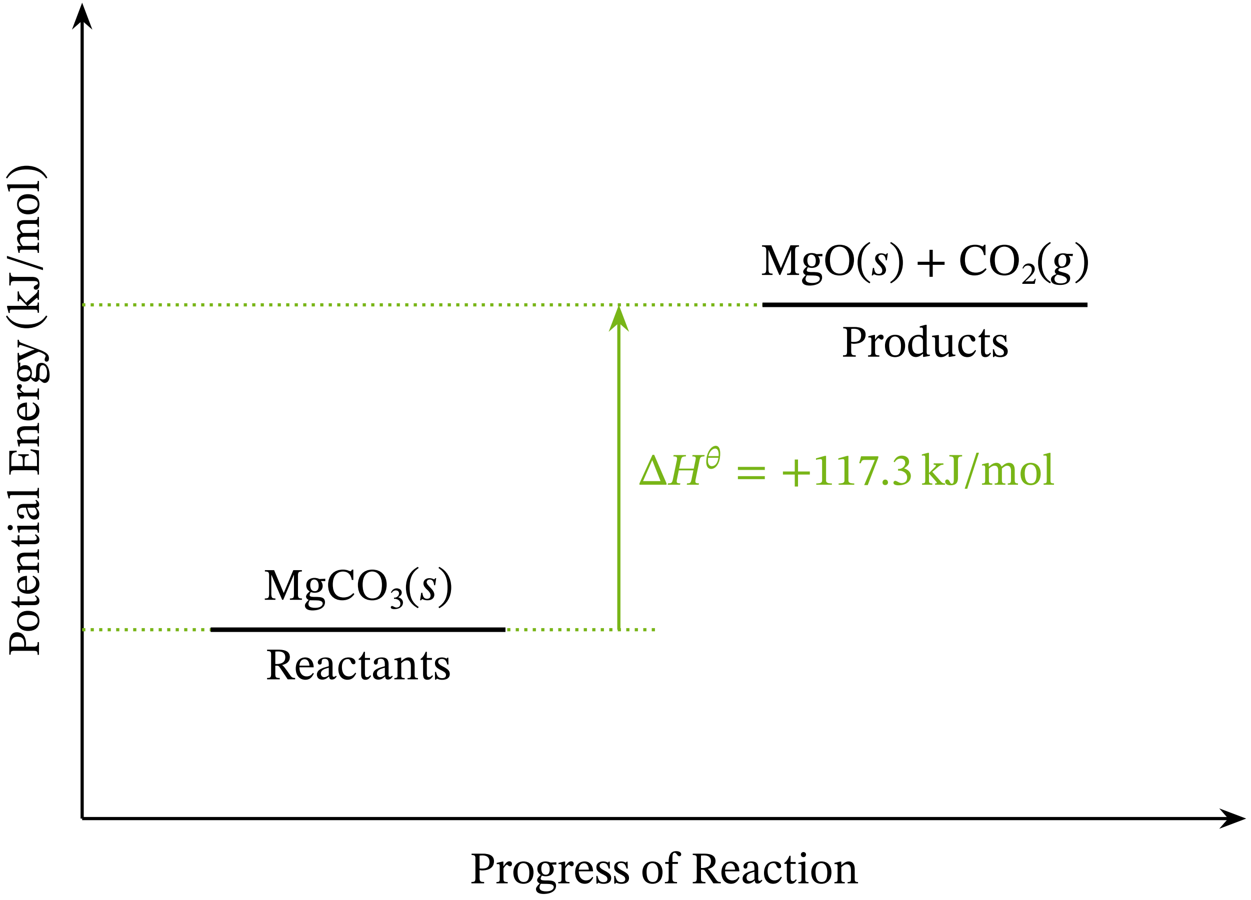
Energy Level Diagram for the Decomposition of Magnesium Carbonate

The thermal decomposition of magnesium carbonate is an endothermic reaction, requiring 117.3 kJ/mol of energy to be absorbed.

The chemical equation for this reaction can be written as

$$MgCO_3(s) + 117.3\,\text{kJ/mol} \longrightarrow MgO(s) + CO_2(g)$$

From the equation and energy level diagram, we can conclude that during the reaction, energy is transferred from the surroundings to the system, so the enthalpy of the products is greater than the enthalpy of the reactants; thus, the change in enthalpy (ΔH) is positive.



Exothermic Reactions

Exothermic chemical reactions release heat energy, and they usually cause the surrounding temperature to increase either slightly or significantly.

In any exothermic chemical reaction, the potential energy of the product molecules is always lower than the potential energy of the reactant molecules.

The products are more stable and less reactive than the reactants.

The enthalpy of the products is lower than the enthalpy of the reactants, and thus the change in enthalpy (ΔH) is negative.

Energy Level Diagram for Exothermic Reactions

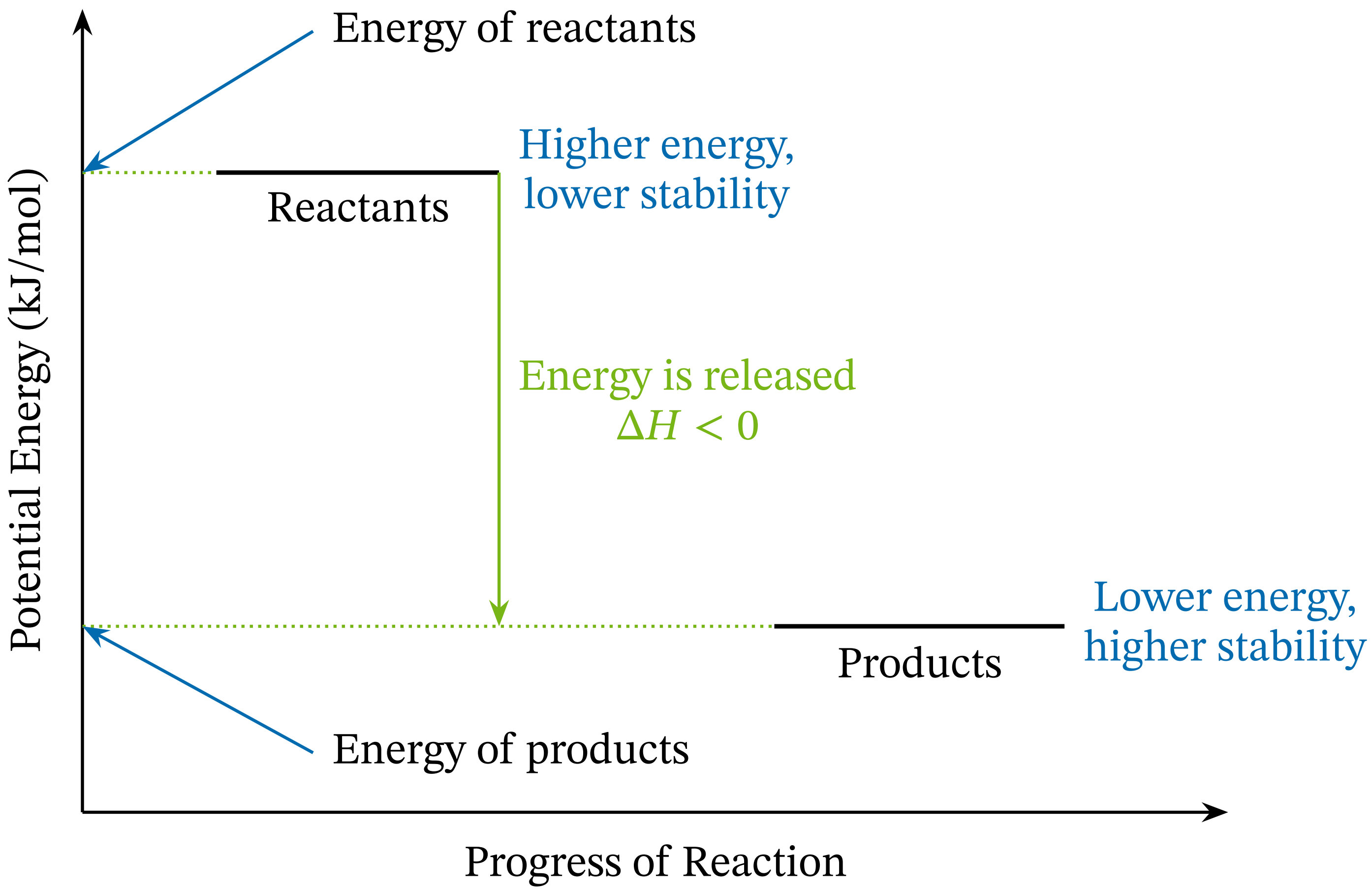
The opposite energy level diagram shows the potential energy of the reactants and the products during a simple exothermic reaction.

The diagram shows that the system releases heat energy as the reaction occurs.

The energy releasing process is represented by the green arrow that stretches from the reactants line to the products line.

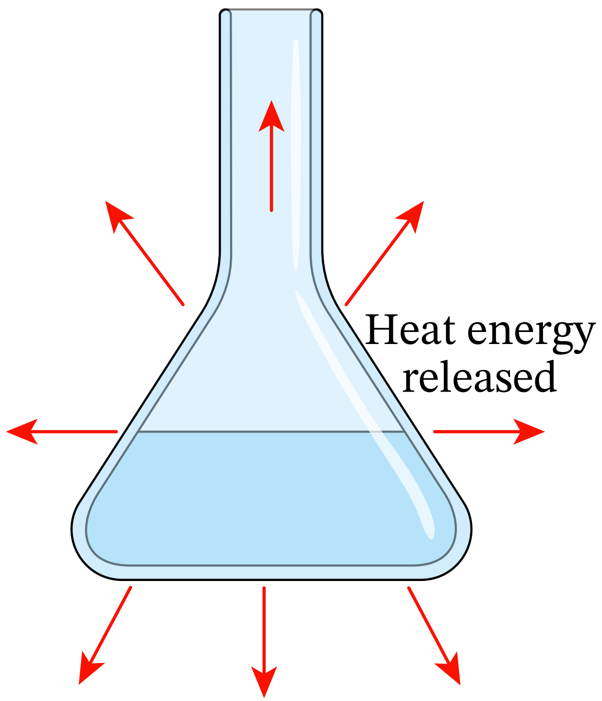
The difference in the energy between the products and the reactants is called the enthalpy change and is given the symbol ΔH:

$\Delta H =$ energy of products $-$ energy of reactants.



Definition of Exothermic Reactions

An exothermic reaction is a chemical reaction where energy is released from the reacting chemicals to the surroundings.



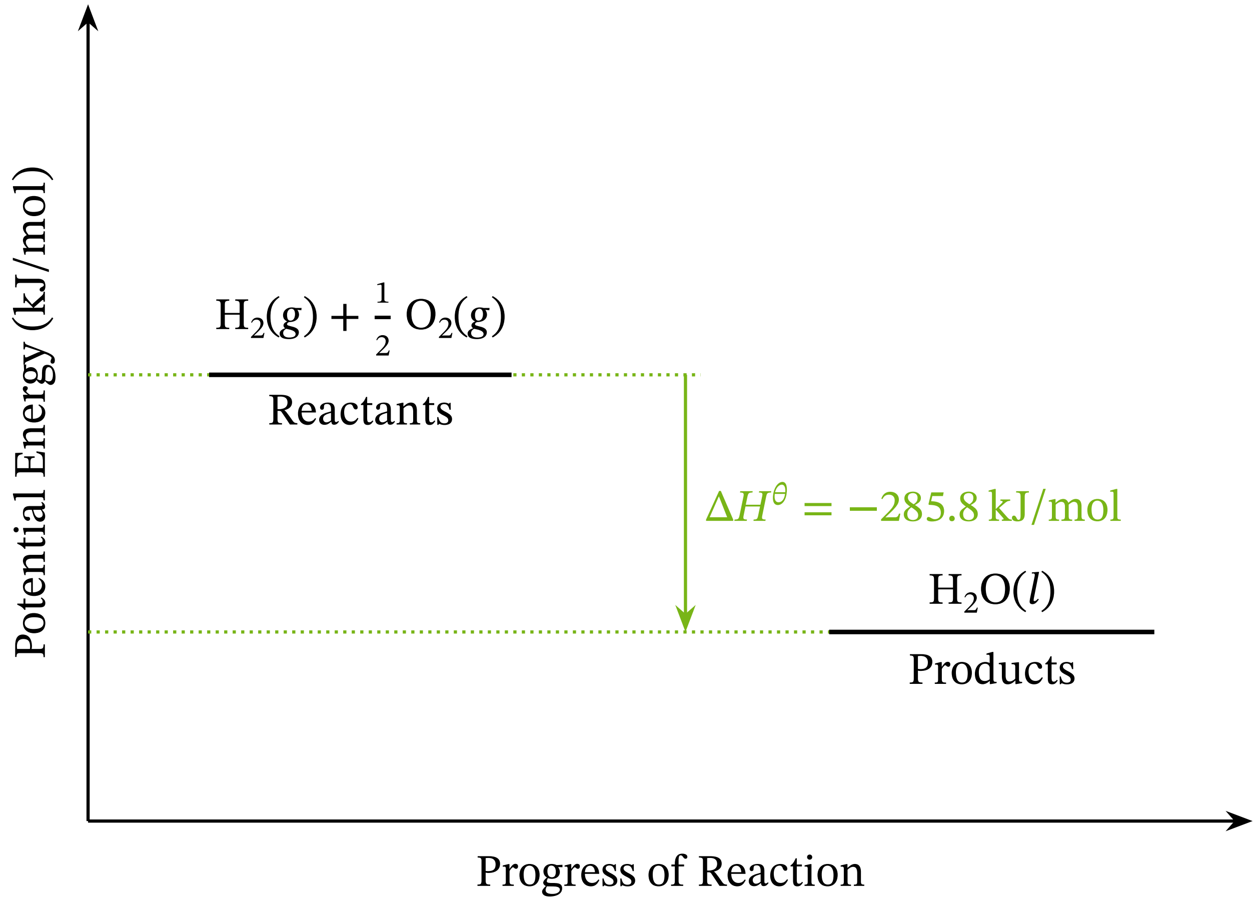
Energy Level Diagram for the Formation of a Water Molecule from Hydrogen and Oxygen

The reaction of hydrogen gas with oxygen gas to produce water is an exothermic reaction, producing 285.8 kJ/mol of energy per mole of hydrogen gas.

The chemical equation for this reaction can be written as

$$H_2(g) + \frac{1}{2}O_2(g) \longrightarrow H_2O(l) + 285.8\ \text{kJ/mol}$$

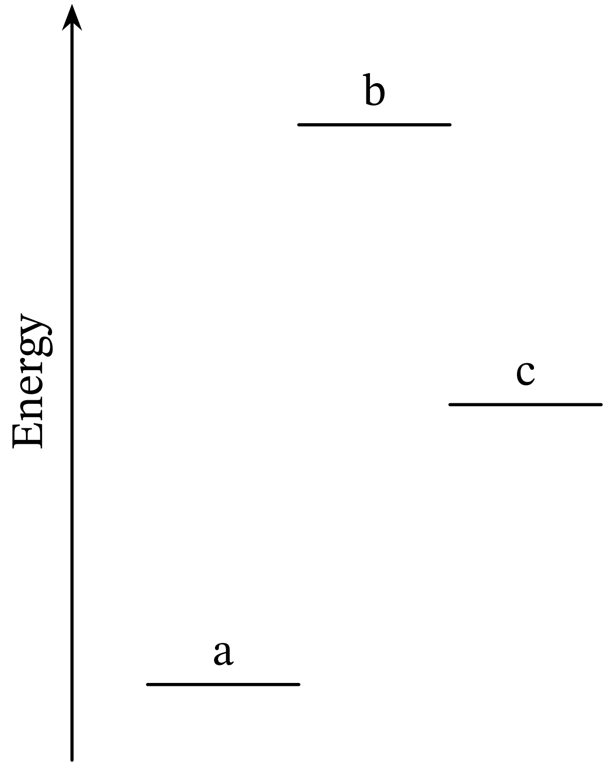
From the equation and energy level diagram, we can conclude that during the reaction, energy is transferred from the system to the surroundings, so the enthalpy of the products is lower than the enthalpy of the reactants; thus, the change in enthalpy (ΔH) is negative.



Example 1: Understanding an Energy Level Diagram

Labeled in the diagram are the chemical energies of three compounds, a–c

1. Which of the labeled compounds is highest in energy?
2. Which of the labeled compounds is lowest in energy?
3. Which of the labeled compounds is most stable?
4. Which of the labeled compounds is least stable?



Example 1 (Continued)

Answer

Part 1

The *y*-axis of an energy level diagram shows the level, or amount, of potential energy stored in a compound.

Different substances have different amounts of potential energy.

Of the three compounds a, b, and c, the one with the highest *y*-axis energy value is compound b. So, the correct answer is b.

Part 2

The compound with the lowest *y*-axis energy value is compound a. The correct answer is a.

Example 1 (Continued)

Part 3

The lower the energy of a compound is, the more stable it is.

When a compound has lower energy, it has high stability and low reactivity.

The compound with the lowest energy is compound a, so compound a is the most stable. The correct answer is a.

Part 4

The higher the energy of a compound is, the less stable it is.

When a compound has higher energy, it has low stability and high reactivity.

The compound with the highest energy is compound b, so compound b is the least stable. The correct answer is b.

Difference between an Energy Level Diagram and a Reaction Profile

Energy level diagrams are simplified illustrations that only show us the initial and final energy of substances during a reaction.

A reaction profile is a more detailed energy level diagram that represents the energy of the substances at different steps during a chemical reaction.

The steps in a reaction include the energy of the reactants and products and the energy pathway for the activated complex or the transition state, which is a high-energy arrangement of atoms, where chemical bonds in the reactants are being broken and new bonds are being formed.

Definition: Reaction Profile

A reaction profile is an energy diagram showing the changes in energy at different steps in a reaction.

Definition: Activated Complex (Transition State)

An activated complex is a high-energy chemical structure where chemical bonds in the reactants are being broken and new bonds are being formed.

The Activated Complex and the Activation Energy

The energy of the activated complex or transition state is equal to the peak energy value of the reaction profile “hump.”

The activated complex has the highest energy of all the substances in a reaction system.

For reactant particles to form an activated complex, they first need to absorb a minimum amount of energy.

This minimum amount of energy required for reactant particles to collide and react with each other is known as the activation energy (E_a).

Definition: Activation Energy (E_a)

Activation energy is the minimum amount of energy required by reactant particles to collide and react with each other.

Chemical Reactions and Activation Energy

Endothermic and exothermic reactions both need activation energy.

This is an initial increase in energy to get the reaction started.

If the energy provided is lower than the activation energy, then there is insufficient energy to start the reaction.

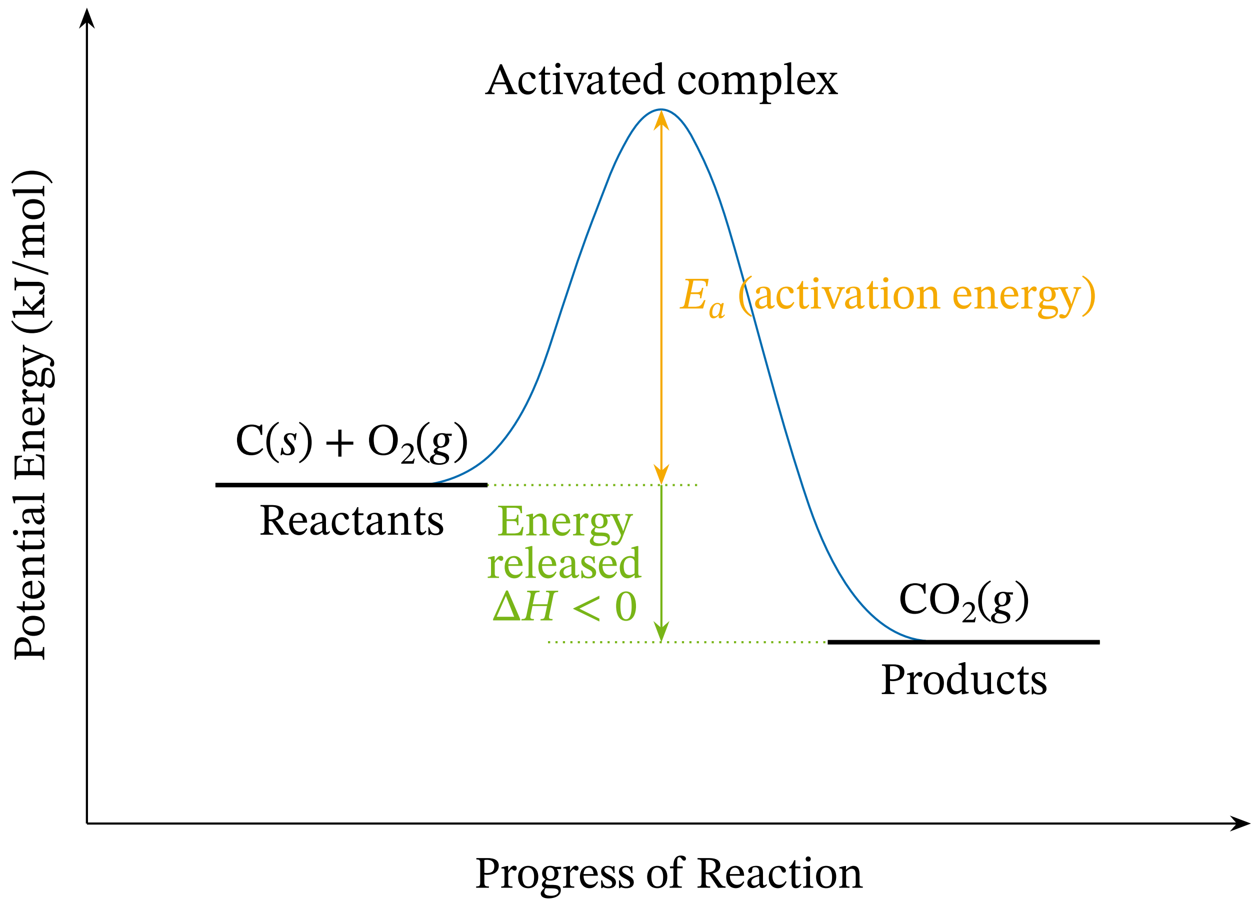
Think of a match; a minimum amount of energy first needs to be absorbed by the system (the chemicals in the match head) to get the reaction started.

This minimum amount of energy is supplied when we strike a match against a rough surface.

The Reaction Profile for an Exothermic Reaction

Let us look at the reaction profile for the reaction between carbon and oxygen gas that produces carbon dioxide gas as the product:

$$C(s) + O_2(g) \longrightarrow CO_2(g) + \text{energy}$$



The Reaction Profile of the Reaction between Carbon and Oxygen to Form Carbon Dioxide

Firstly, we can see that the reaction is exothermic because the energy of the product, CO_2(g), is lower than the energy of the reactant molecules.

We can see a “hump” in the diagram starting at the energy level of the reactants and ending at the energy level of the products.

The orange arrow represents the activation energy or how much energy is required to break the covalent bonds that hold the reactant molecules together.

Energy is released by the reactants to form the products, and ΔH is therefore negative.

The Activation Energy and Catalysts

One way to reduce the activation energy of this reaction would be to use a catalyst.

This is because catalysts act by lowering the activation energy needed for a reaction to occur and, in this way, catalysts can speed up a reaction.

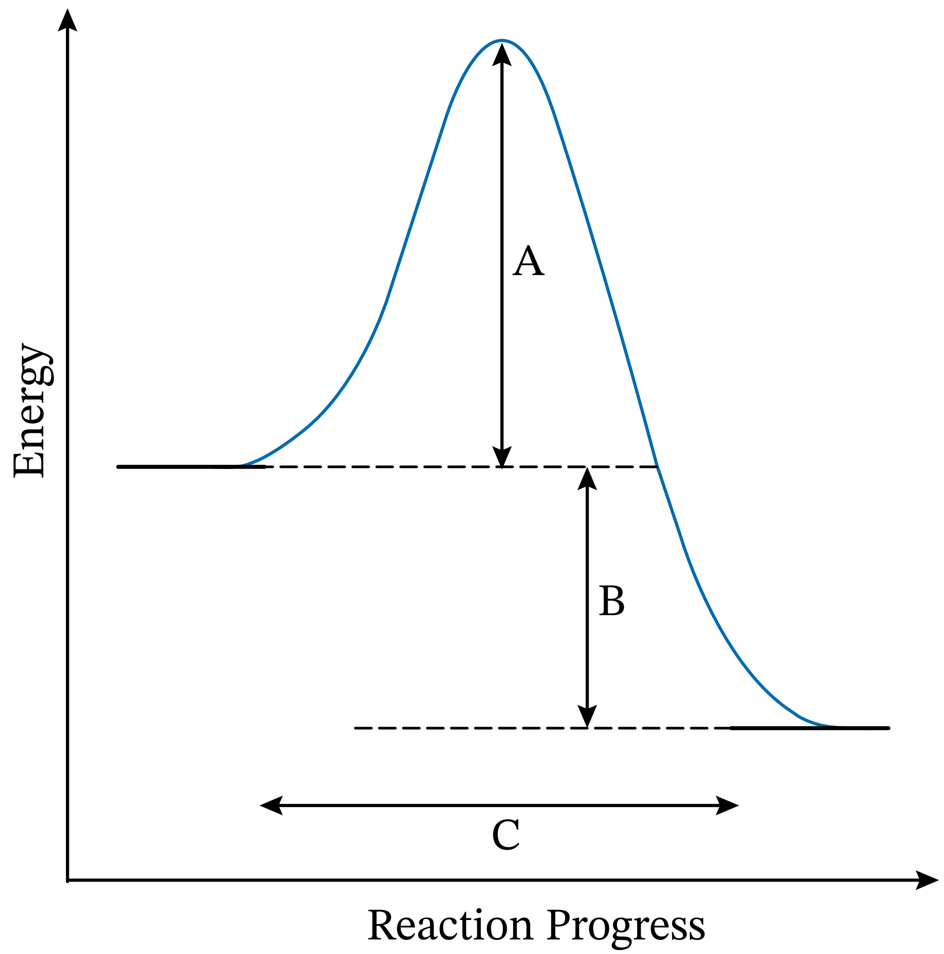
Catalysts do not take part in chemical reactions, and they do not undergo chemical changes themselves.

Definition: Catalyst

A catalyst is a substance that increases the rate of a chemical reaction, without being chemically altered itself, by lowering the activation energy needed for the reaction to occur.

Example 2: Identifying Which Part of a Reaction Profile Corresponds to Activation Energy

The reaction profile for a chemical reaction is shown in the diagram below. Which label corresponds to the activation energy?



Example 2 (Continued)

Answer

The activation energy is the minimum amount of energy required to cause the reactants to collide and react with each other.

So, whether a reaction is endothermic or exothermic, the reactants must initially absorb enough energy to react.

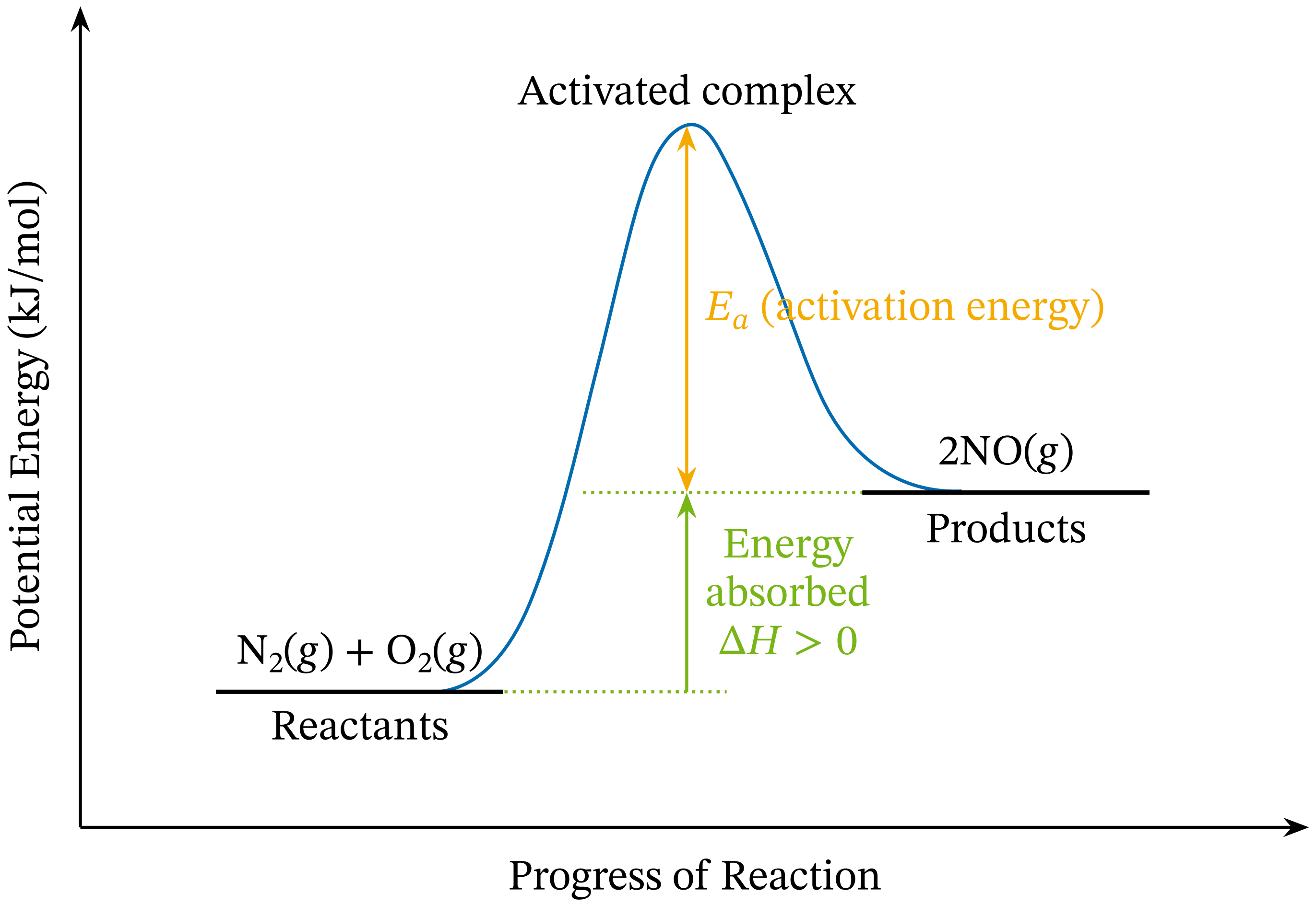
Activation energy on a reaction profile is the initial energy increase by the reactants.

This corresponds to A.

The Reaction Profile for An Endothermic Reaction

Let us look at the reaction profile for the endothermic reaction between nitrogen gas and oxygen gas:

$$N_2(g) + O_2(g) + \text{energy} \longrightarrow 2\,NO(g)$$



The Reaction Profile of the Reaction between Nitrogen and Oxygen to Form Nitric Oxide

Firstly, we can see that the reaction is endothermic because the energy of the product, NO(g), is higher than the energy of the reactant molecules.

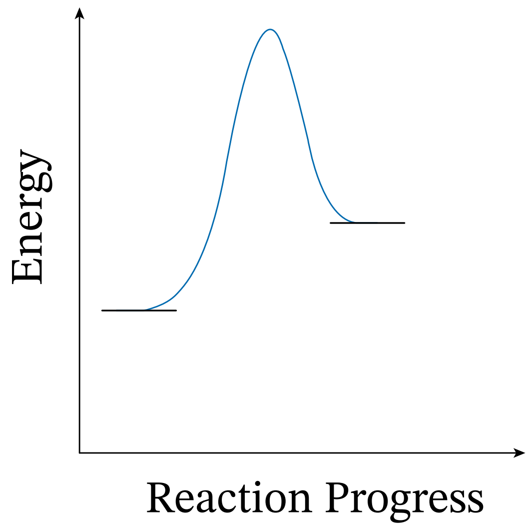
We can see a “hump” in the diagram starting at the energy level of the reactants and ending at the energy level of the products.

The orange arrow represents the activation energy or how much energy is required to break the covalent bonds that hold the reactant molecules together.

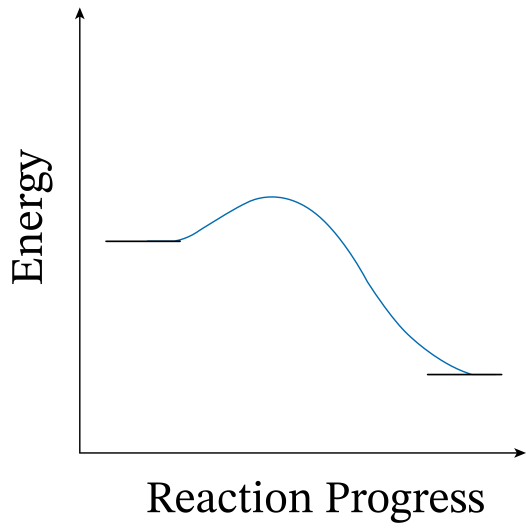
Energy is absorbed by the reactants to form the products, and ΔH is therefore positive.

Example 3: Selecting the Correct Reaction Profile Diagram from Information Given about a Reaction

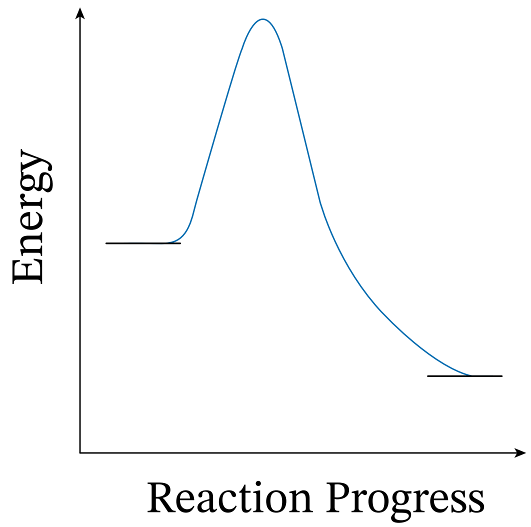
A chemical reaction is found to have a molar reaction enthalpy (ΔH) of -80 kJ/mol and an activation energy of 25 kJ/mol. Which of the following reaction profiles represents this reaction?



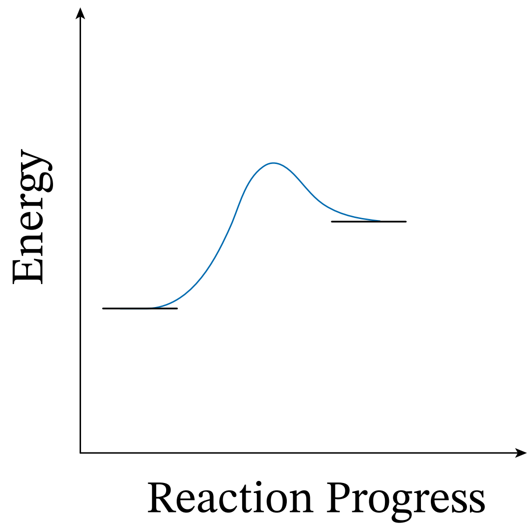
(A)



(B)



(C)



(D)

Example 3 (Continued)

Answer

We are told that the enthalpy change of the reaction is $-80\ \text{kJ/mol}$. Because ΔH is negative, we know the reaction is exothermic.

Only options B and C represent exothermic reactions. So, we can rule out A and D.

We can compare the reaction profiles in answers B and C. We can see that in answer C, the vertical distance between the reactants and products energy lines (ΔH) is almost the same as the vertical distance between the reactant energy line and the top of the curve where the activated complex is, in other words, the activation energy. But this is not the case for B.

Example 3 (Continued)

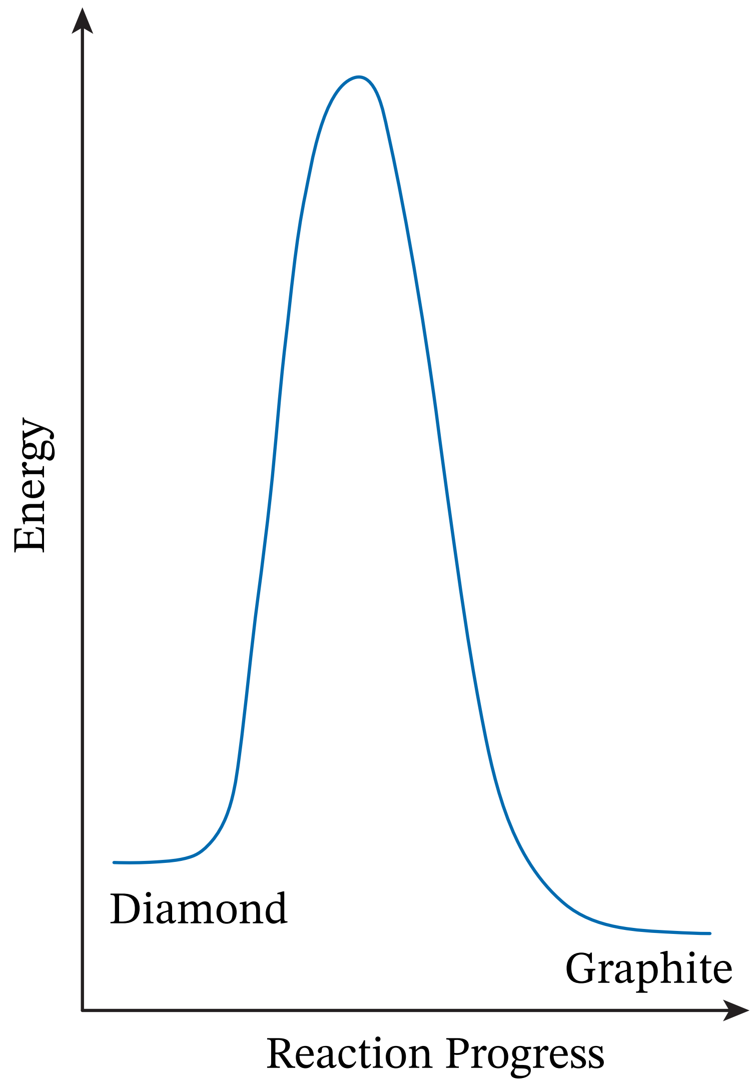
In other words, in reaction profile C, ΔH is approximately equal to the activation energy E_a. So, we can rule out option C as the answer, because we know that $\Delta H = -80\,\text{kJ/mol}$ and $E_a = 25\,\text{kJ/mol}$; ΔH and E_a are not equal.

When we look at answer option B, we can see that E_a is approximately a third of the height that ΔH is.

So, the correct answer is B.

Example 4: Interpreting a Reaction Profile

The reaction profile diagram below shows that graphite is more stable than diamond. However, the conversion from diamond to graphite is very difficult. Which of the following statements explains why?



A. Diamond does not conduct electricity.

B. The energy required to break the covalent bonds between carbon atoms is low.

C. The reaction is exothermic, not endothermic.

D. The energy difference between diamond and graphite is very small.

E. The activation energy for the conversion of diamond into graphite is very high.

Example 4 (Continued)

Answer

In the question, we are told that graphite is more stable than diamond.

The reaction profile indicates that the conversion of diamond to graphite is an exothermic process as the relative energies of the reactant (diamond) are higher than those of the product (graphite).

Statement C, “the reaction is exothermic, not endothermic,” is a correct statement for this reaction but does not fully answer the question.

Example 4 (Continued)

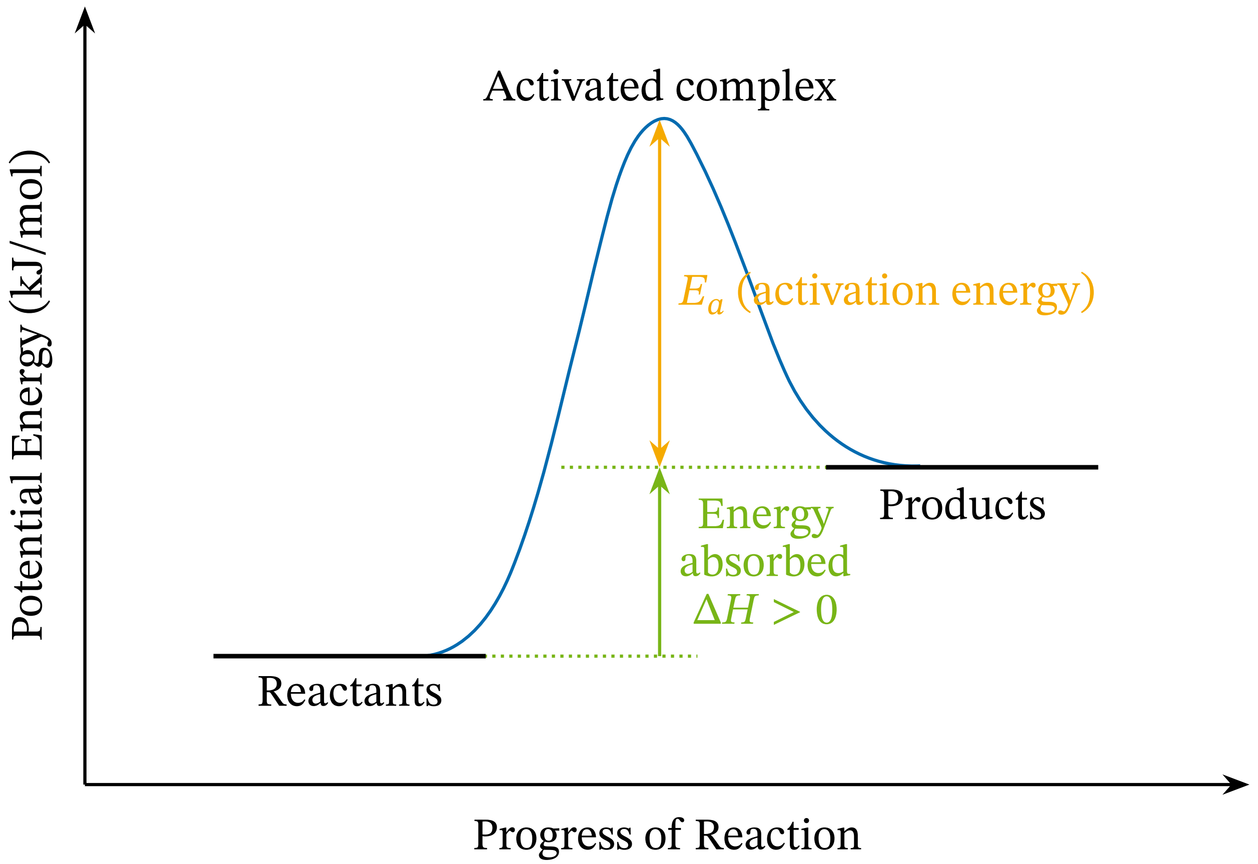
Although the energies of diamond and graphite are not greatly different (their energy values on the reaction profile are relatively close to each other), the "hump" for the activation energy required to induce diamond to react and be converted to graphite is relatively large.

This tells us that it takes a lot of energy to convert diamond to graphite. So, although statement D, "the energy difference between diamond and graphite is very small," is also a correct description of this reaction profile, it is not the reason why it is so difficult to convert diamond to graphite.

The reason why it is so difficult is the very large amount of activation energy that would be required for this reaction to occur. So, the correct answer is E: the activation energy for the conversion of diamond into graphite is very high.

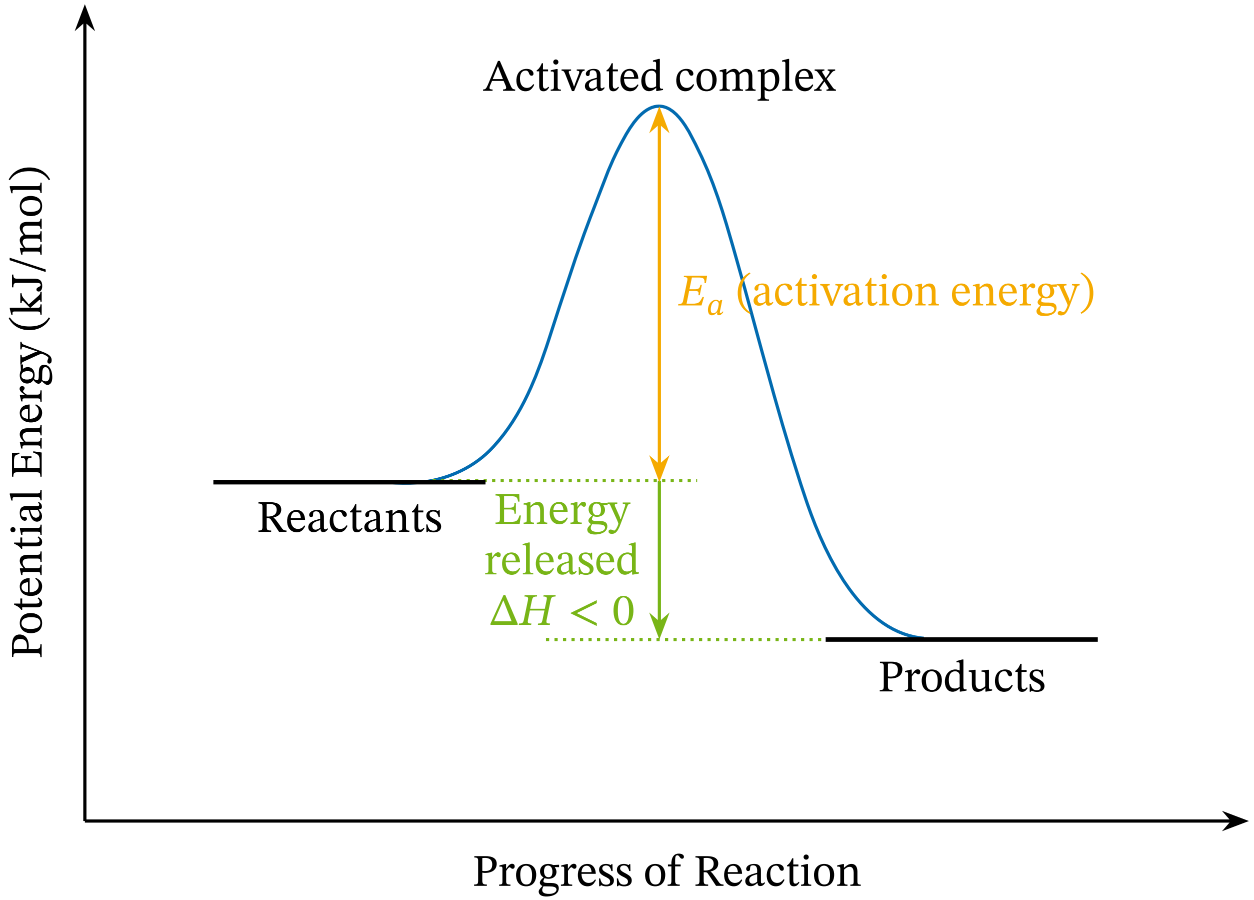
Key Points

- A reaction profile shows the amount of energy at different steps in a reaction.
- A typical endothermic reaction profile looks as shown below.



Key Points (Continued)

- A typical exothermic reaction profile looks as shown below.



Key Points (Continued)

- A high-energy substance has low stability, and a low-energy substance has high stability.
- An activated complex is a high-energy state of chemical structures where chemical bonds in the reactants are being broken and new bonds are being formed.
- The activation energy (E_a) is the minimum amount of energy that reactants need to collide and react.
- The enthalpy change (ΔH) is the difference in energy between the products and the reactants.