

Bond Energy

What makes a reaction endothermic or exothermic?

Why?

Chemical reactions can be a lot like playing with Legos®—you must take apart part of your last creation before you can replace it with something new. For many chemical reactions, we have to first break bonds in the reactants before we can put the atoms back into a new arrangement to form the products. Both of these processes involve changes in energy. The net energy change for a reaction is called the **heat of reaction** or the **change in enthalpy** (ΔH). In this activity we will look at one way energy changes can be approximated for chemical reactions.

Model 1 – Breaking and Forming Bonds

	Reaction	Change in Energy (kJ/mol _{rxn})		Reaction	Change in Energy (kJ/mol _{rxn})
A)	$\text{PCl}_3(\text{g}) \rightarrow \text{P}(\text{g}) + 3\text{Cl}(\text{g})$	+ 966.7 <i>broken</i>	E)	$\text{P}(\text{g}) + 3\text{Cl}(\text{g}) \rightarrow \text{PCl}_3(\text{g})$	- 966.7 <i>formed</i>
B)	$\text{PCl}_5(\text{g}) \rightarrow \text{P}(\text{g}) + 5\text{Cl}(\text{g})$	+ 1,297.9 <i>broken</i>	F)	$\text{P}(\text{g}) + 5\text{Cl}(\text{g}) \rightarrow \text{PCl}_5(\text{g})$	- 1,297.9 <i>formed</i>
C)	$\text{PF}_3(\text{g}) \rightarrow \text{P}(\text{g}) + 3\text{F}(\text{g})$	+ 1,470.4 <i>broken</i>	G)	$\text{P}(\text{g}) + 3\text{F}(\text{g}) \rightarrow \text{PF}_3(\text{g})$	- 1,470.4 <i>formed</i>
D)	$\text{PF}_5(\text{g}) \rightarrow \text{P}(\text{g}) + 5\text{F}(\text{g})$	+ 2,305.4 <i>broken</i>	H)	$\text{P}(\text{g}) + 5\text{F}(\text{g}) \rightarrow \text{PF}_5(\text{g})$	- 2,305.4 <i>formed</i>

- Identify four reactions in Model 1 where bonds are being broken. Write "broken" in the Change in Energy box in the table for each reaction you identify.
- Identify four reactions in Model 1 where bonds are being formed. Write "formed" in the Change in Energy box in the table for each reaction you identify.
- Circle the correct word to complete each sentence below.
 - When bonds are (broken/formed) there is a positive energy change.
 - Breaking bonds is (endothermic/exothermic).
 - When bonds are (broken/formed) there is a negative energy change.
 - Forming bonds is (endothermic/exothermic).
- Find two reactions in Model 1 that are exact opposites of each other, that is, one reaction is the reverse of the other reaction.
 - How do the changes in energy for the reverse reactions compare?

The changes in energy for these reactions are the same, but opposite in sign.
 - Explain your answer to part a considering what you learned from Questions 1–3 about bond breaking and bond formation.

If a given amount of energy is required to break a bond, then the same amount of energy will be released when the bond is formed.

Bond Energy Pogil Model 4

Ying-Ying Zheng



Bond Energy Pogil Model 4:

Organic Chemistry Suzanne M. Ruder, The POGIL Project, 2015-12-29 ORGANIC CHEMISTRY *Empirical Methods for Calculation of Bond Energies* Hans H. Jaffé, Van Tran Zung, United States. Air Force. Systems Command. Aeronautical Systems Division, University of Cincinnati, 1961 **Bond Dissociation Energies of Energetic Compounds: A**

Comparison of Theoretical Methods, 2000 Due to their computational efficiency density functional methods utilizing semiempirical hybrid functionals such as B3LYP are commonly used in calculating the molecular potential energy surfaces of a wide variety of molecules In particular potential energy surfaces of several energetic compounds such as hexahydro 1 3 5 trinitro 1 3 5 triazine RDX 1 3 3 trinitroazetidine TNAZ 5 nitro 2 4 dihydro 3H 1 2 4 triazolone NTO and 1 1 diamino 2 2 dinitroethylene recently have been computed using density functional methods B3LYP These potential energy surfaces are used for example to predict the decomposition mechanisms and for constructing force fields for modeling and simulation of solid state phase transitions The accuracy of B3LYP relative energies and structures is generally observed to be comparable to that obtained using second order perturbation theory methods However an unresolved issue is the reliability of density functional based methods in cases where a significant degree of multiconfigurational character may be present in the compounds of interest such as in the energetic molecules listed above The present study is a systematic comparison of several electronic structure methods in the prediction of bond dissociation energies of energetic molecules In particular the C NO₂ and C NH₂ bond dissociation energies of 1 1 diamino 2 2 dinitroethylene and its prototypes are used as a testbed for comparison of B3LYP with single configuration self consistent field SCF second order perturbation theory MP2 and coupled cluster CCSD T calculations as well as multiconfigurational SCF MCSCF and quasi dependent perturbation theory MCQDPT methods **The Energy-energy Correlation Function of the Random Bond Ising Model in Two Dimensions** Klaus

Ziegler, 1993 **Empirical Bond Energies** FRANK JR. WILSON, AIR FORCE FLIGHT TEST CENTER EDWARDS AFB CALIF., Air Force Flight Test Center (U.S.), 1961 A consistent set of bond energy values are calculated on the assumption that bond energy nonconstancies are a minimum when determined from compounds in which all the constituent elements exhibit their normal valency Several empirical rules for estimating the heats of vaporization and fusion are included The report contains sufficient data for the estimation of heats of formation of compounds In many cases estimations can be made within a few kilocalories Author

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