

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.

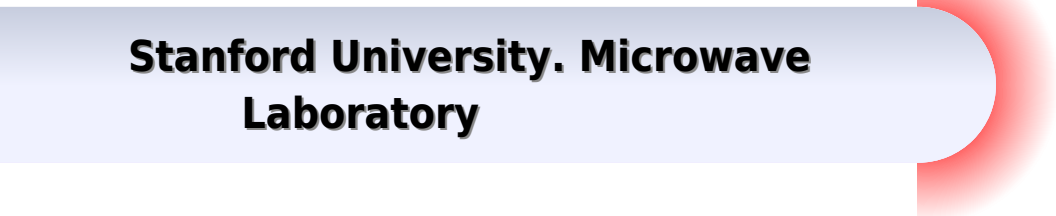
- Explain your answer to part a considering what you learned from Questions 1–3 about bond breaking and bond formation.

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.



Pogil Bond Energy Key 2

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Analytical Chemistry Juliette Lantz, Renée Cole, The POGIL Project, 2014-12-31 An essential guide to inquiry approach instrumental analysis Analytical Chemistry offers an essential guide to inquiry approach instrumental analysis collection The book focuses on more in depth coverage and information about an inquiry approach This authoritative guide reviews the basic principles and techniques Topics covered include method of standard the microscopic view of electrochemistry calculating cell potentials the BerriLambert atomic and molecular absorption processes vibrational modes mass spectra interpretation and much more Calculation of the Bond Energy and Bond Length of the N₂ Molecule Via the Hartree-Fock and the DMRG Method Chiara Sommer, 2018 **Bond Orbital Model 2** Stanford University. Microwave Laboratory, 1974

Strong Bond Activation Using Rhodium Yunzhe Jiao, 2014 The reactive fragment Tp Rh L where Tp tris 3 5 dimethylpyrazolyl borate and L isocyanide or phosphine has been used in C H activation of hydrocarbons The first study in chapter 2 examines C H bond activation of molecules with alpha substitution to form the type of products Tp Rh CNneopentyl CH₂X H where X CH₂C O CH₃ H₂C triple bond CCH₃ CH₂O t Bu CH₂CF₃ CH₂F and CHF₂ Relative rhodium carbon bond energies are measured from competition and reductive elimination experiments Two separate linear correlations are observed between Rh C and C H bond energies The substituted group are stabilized by 7.5 kcal/mol relative to the parent hydrocarbons The effect of the substituent could be attributed to the hyperconjugation or inductive effects which increase the charge distribution in the Rh C bond As the Rh CH₂X bond except X F Cl is weaker relative to Rh CH₃ bond the product selectivity in branched vs linear olefin insertion is determined by the formation of beta C H bond The effect of the spectator ligand in C H bond activation is investigated The first example of ligand variation is the replacement of a pi acceptor isonitrile spectator ligand with a sigma donor phosphine spectator in the Tp Rh L fragment chapter 3 A wide scope of aliphatic aromatic alkenylic and alkynylic C H bonds are activated to give the type of products Tp Rh PMe₃ R H Like the Tp Rh CNR system the substituted hydrocarbons also have a distinct correlation from the parent group but the correlations of bond energies in Tp Rh PMe₃ R H are noticeably different from the isocyanide analog The ligand effect in thermodynamics of C H activation is quantified by comparing the two systems In a similar study the Tp Rh P OMe₃ fragment is used to activate of sp³ sp² and sp C H bonds which gives us a better understanding of ligand effects on metal carbon bond strengths chapter 4 Two distinct linear correlations based on alpha substitution are once again shown in the phosphite system Generally the slope values for the alpha unsubstituted group in Tp Rh PR₃ R H R Me OMe are close and they are both larger than that in Tp Rh CNneopentyl R H 1.38 For stabilized M C bonds the slope change follows an order of Tp Rh PMe₃ 1.71 Tp Rh P OMe₃ 1.45 Tp Rh CNneopentyl 1.40 This trend is consistent with the decrease of electronic density around the rhodium center which means Rh C bond strengths are more separated in a more electronic rich and crowded system The work in chapter 5 shows the reactivities of the Tp Rh PMe₃ fragment in activation of chlorohydrocarbons at ambient temperature C H

activation is kinetically preferred while the thermally stable products were formed from C Cl cleavage and or beta chloride elimination In the previous work the metal fragment Tp Rh CNR with a pi acceptor ligand showed exclusive selectivity for C H activation of chloromethane and no evidence for C Cl activation DFT calculations are utilized to study the energetics for C H and C Cl bond activation of chloromethane by Tp Rh PMe₃ vs Tp Rh CNMe A plausible C Cl activation pathway is associated with the generation of a methyldiene intermediate after losing the spectator ligand The ligand dissociation energy is likely to be the key factor in determining the activation barrier for C Cl bond cleavage To continue with the activation of hydrocarbons containing functional groups the activation of alcohols by Tp Rh PMe₃ was also studied chapter 6 The series of linear alcohols and water gives exclusive activation of the O H bonds In activation of branched alcohols the formation of a species Tp Rh PMe₃ OH H is observed presumably via beta OH elimination of the non observable C H activation intermediates The clean reductive eliminations of ROH from Tp Rh PMe₃ OR H and the competition experiments allows the determination of relative Rh O bond energies The correlation of Rh O vs O H bond energies demonstrates a good linearity with a slope of 0.87 for unsubstituted alcohols and water The involvement of electron withdrawing groups such as fluorine or a hydroxyl tends to strengthen the Rh O bond compared to their corresponding O H bond Pages vii viii

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

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