Enthalpy and The First Law DCI

Name S	ection	
1 Energy in the form of heat can be either released (exothermic) or absorbed (endothermic) in a chemical reaction. The heat, called enthalpy, is a driving force for chemical reactions. Predict which of the following thermodynamically favored reactions are exothermic and which are endothermic.		
a) $H_2O(l) \rightarrow H_2O(g)$ at 25 °C	endothermic	
b) $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$	exothermic	
c) $Ba(OH)_2 \cdot 8H_2O(s) + 2NH_4Cl(s) \rightarrow BaCl_2(aq) + 2NH_3(g) + 10H_2O(s)$	(l) endothermic	
d) $H_2(g) + \frac{1}{2}O_2(g) \to H_2O(l) \text{ or } (g)$	exothermic	
e) $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$	exothermic	
f) $Al(s) + \frac{3}{2}Br_2(l) \rightarrow AlBr_3(s)$	exothermic	

2. A formation reaction is a chemical reaction depicting the formation of one mole of a substance from its naturally occurring elemental sources. Which of the reactions in question 1 are formation reactions?

A formation reaction is characterized as having elements in their standard states forming 1 mol of product.

So d and f are both formation reactions.

d)
$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l) \text{ or } (g) \text{ and } f) Al(s) + \frac{3}{2}Br_2(l) \rightarrow AlBr_3(s)$$

However, b is NOT a formation reaction

b) $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$

The reactants are in their standard state, however 2 moles of product are formed. For this reaction to be a formation reaction the equation would have to be;

$$Mg(s) + \frac{1}{2}O_2(g) \rightarrow MgO(s)$$

3. A table of enthalpies of formation, $\Delta H_{\mathbf{f}}^{\circ}$, for selected substance is at the end of this DCI. Write the mathematical equation which relates the standard heat of reaction to the heats of formation of the reactants and products of the chemical reaction.

The heat (enthalpy) of reaction can be determined by adding together the enthalpies of formation associated with a series of formation reactions which can generate the desired reaction.

 $\Delta H_{rxn}^{\circ} = \Sigma m \Delta H_{f}^{\circ} \text{ (products)} - \Sigma n \Delta H_{f}^{\circ} \text{ (reactants)}$

- 4. Calculate $\Delta H^{\circ}_{reaction}$ for the following chemical reactions.
- a) $H_2O(l) \rightarrow H_2O(g)$ at 25 °C (note: this reaction is NOT thermodynamically favored at 25 °C)

 $\Delta H_{rxn}^{\circ} = +44 \text{ kJ mol}^{-1}$

b) $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$

 $\begin{array}{ll} \Delta H_{rxn}^{\circ} &= -1202 \ kJ \ mol^{-1} \\ c) & Ba(OH)_2 \cdot 8H_2O(s) + 2NH_4Cl(s) \rightarrow BaCl_2(aq) + 2NH_3(g) + 10H_2O(l) \\ \Delta H_{rxn}^{\circ} &= \Sigma m \Delta H_{\ f}^{\circ} \ (products) \ - \Sigma n \Delta H_{\ f}^{\circ} \ (reactants) \\ &= \Delta H_{\ f}^{\circ} \ (BaCl_2) + 2\Delta H_{\ f}^{\circ} \ (NH_3) + 10\Delta H_{\ f}^{\circ} \ (H_2O) \\ & - (\Delta H_{\ f}^{\circ} \ (Ba(OH)_2 \cdot 8H_2O) \ + 2\Delta H_{\ f}^{\circ} \ (NH_4Cl) \) \\ &= (-872 \ kJ \ mol^{-1}) + 2(-46 \ kJ \ mol^{-1}) + 10(-286 \ kJ \ mol^{-1}) \ - \ ((-3342 \ kJ \ mol^{-1}) \ + 2(-314 \ kJ \ mol^{-1})) \\ &= (-872 \ kJ \ mol^{-1} + (-92 \ kJ \ mol^{-1}) + (-2860 \ kJ \ mol^{-1})) \ - \ (-3342 \ kJ \ mol^{-1} + (-628 \ kJ \ mol^{-1})) \\ &= 146 \ kJ \ mol^{-1} \end{array}$

d) $H_{2(g)} + \frac{1}{2}O_{2(g)} \rightarrow H_{2}O(l)$ or (g) $\Delta H_{rxn}^{\circ} = -286 \text{ kJ mol}^{-1}$ for the liquid phase and -242 kJ mol^{-1} for the gas

phase

e)
$$CH_{4(g)} + 2O_{2(g)} \rightarrow CO_{2(g)} + 2H_{2}O(l)$$

 $\Delta H_{rxn}^{\circ} = \Sigma m \Delta H_{f}^{\circ} \text{ (products)} - \Sigma n \Delta H_{f}^{\circ} \text{ (reactants)}$
 $= (\Delta H_{f}^{\circ} (CO_{2}) + 2\Delta H_{f}^{\circ} (H_{2}O)) - (\Delta H_{f}^{\circ} (CH_{4}) + 2\Delta H_{f}^{\circ} (O_{2}))$
 $= [(-393.5 \text{ kJ mol}^{-1}) + (-285.8 \text{ kJ mol}^{-1})] - [(-74.8 \text{ kJ mol}^{-1}) + (0)]$
 $= -890 \text{ kJ mol}^{-1}$

f)
$$\operatorname{Al}(s) + \frac{3}{2}\operatorname{Br}_{2}(l) \to \operatorname{AlBr}_{3}(s)$$

 $\Delta H_{\mathbf{rxn}}^{\circ} = \Sigma m \Delta H_{\mathbf{f}}^{\circ} (\operatorname{products}) - \Sigma n \Delta H_{\mathbf{f}}^{\circ} (\operatorname{reactants})$
 $= \Delta H_{\mathbf{f}}^{\circ} (\operatorname{AlBr}_{3}) - [\Delta H_{\mathbf{f}}^{\circ} (\operatorname{Al}) + \frac{3}{2} \Delta H_{\mathbf{f}}^{\circ} (\operatorname{Br}_{2})]$
 $= (-526.3 \text{ kJ mol}^{-1}) - [(0) + \frac{3}{2} (0)] = -526.3 \text{ kJ mol}^{-1}$

4. The natural tendency for spontaneous chemical reactions is to release heat. Is enthalpy an absolute predictor of thermodynamically favorability?

No, enthalpy is not an absolute predictor of whether a reaction is thermodynamically favored.

Substance	ΔH_{f}°	Substance	ΔH_{f}°
and State	(kJ/mol)		<u>(kJ/mol)</u>
C(s) (graphite)	0	HCl(g)	-92.3
C(s) (diamond)	2	$\operatorname{HBr}(g)$	-36.4
CO(g)	-110.5	$\operatorname{HI}(g)$	26.5
$CO_2(g)$	-393.5	$I_2(g)$	62.25
$CH_4(g)$	-75	$O_2(g)$	0
$CH_3OH(g)$	-201	$\mathrm{O}(g)$	249
$CH_3OH(l)$	-239	$O_3(g)$	143
$H_2CO(g)$	-116		
$\text{CCl}_4(l)$	-135.4	$N_2(g)$	0
HCOOH(g)	-363	$NH_3(g)$	-46
HCN(g)	135.1	$NH_3(aq)$	-80
$CS_2(g)$	117.4	$NH_4^+(aq)$	-132
$CS_2(l)$	89.7	$NH_4Cl(s)$	-314.4
$C_2H_2(g)$	227	$N_2H_4(l)$	50.6
$C_2H_4(g)$	52	NO(g)	90.25
$CH_3CHO(g)$	-166	$NO_2(g)$	33.18
$C_2H_5OH(l)$	-278	$N_2O(g)$	82.0
$C_2H_5O_2N(g)$	-533	$N_2O_4(g)$	9.16
$C_2H_6(g)$	-84.7	$N_2O_4(l)$	20
$C_{3}H_{6}(g)$	20.9	$HNO_3(aq)$	-207.36
$C_3H_8(g)$	-104	$HNO_3(l)$	-174.10
$C_{4}H_{10}(g)$	-126	$NH_4ClO_4(s)$	-295
$C_8H_{18}(l)$	-208	,	
$CH_2 = CHCN(l)$	152		
$CH_3COOH(l)$	-484	$S_2Cl_2(g)$	-18
$C_{6}H_{12}O_{6}(s)$	-1275	$SO_2(g)$	-296.83
0 12 0()		$H_2S(g)$	-20.6
$\operatorname{Cl}_2(g)$	0	$SOCl_2(g)$	-213
$Cl_2(aq)$	-23	_ (0)	
$Cl^{-}(aq)$	-167.5	SiCl _{4(g)}	-657
		$SiO_{2}(s)$	-910.94
		$SiF_{4(g)}$	-1614.9
$H_{2(g)}$	0		
H(g)	217	$Ba(OH)_2 \cdot 8H_2O(s)$	-3342
$\mathrm{H}^{+}(aq)$	0	$BaCl_{2}(aq)$	-872
OH ⁻ (aq)	-230	AlBr ₃ (s)	-526
$H_2O(l)$	-286	5/~/	-
$H_2O(g)$	-242	ZnS(s)	-206