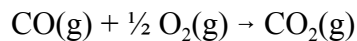


For the reaction



the following data taken from Schaum's, NBS Tables, JANAF Tables, and NIST will be of value for Questions 1-4.

$\overline{\text{BE}}/(\text{kJ mol}^{-1})$	C	O	
O -	326	142	
O =	803 ^a	498	^a 728 if R ₁ R ₂ C = O
O ≡	1075	----	
C -	331		
C =	590 ^c		^c 506 if alternating - and =
C ≡	812		

	O ₂ (g)	CO(g)	CO ₂ (g)
$\Delta_f H_{298}^\circ/(\text{kJ mol}^{-1})$		-110.525	-393.509
$\Delta_f G_{298}^\circ/(\text{kJ mol}^{-1})$		-137.168	-394.359
$(H_{298}^\circ - H_0^\circ)/(\text{kJ mol}^{-1})$	8.680	8.665	9.360
$(H_{1000}^\circ - H_0^\circ)/(\text{kJ mol}^{-1})$	31.386	30.361	42.761
$S_{298}^\circ/(\text{J K}^{-1} \text{mol}^{-1})$	205.138	197.674	213.74
$A/(\text{J K}^{-1} \text{mol}^{-1})$	29.65900	25.56759	24.99735
$B/(10^{-3} \text{J K}^{-2} \text{mol}^{-1})$	6.137261	6.096130	55.18696
$C/(10^{-6} \text{J K}^{-3} \text{mol}^{-1})$	-1.186521	4.054656	-33.69137
$D/(10^{-9} \text{J K}^{-4} \text{mol}^{-1})$	0.095780	-2.671301	7.948387
$E/(10^6 \text{J K mol}^{-1})$	-0.219663	0.131021	-0.136638

For O₂(g): g(elec) = 3, $\tilde{\nu} = 1580.1932 \text{ cm}^{-1}$; $I = 1.936398 \times 10^{-46} \text{ kg m}^2$

1(15). Using the average bond enthalpy data, estimate $\Delta_r H^\circ_{298}$.

Why is this value only an estimate?

Using $\Delta_r H^\circ_{298}$ data, calculate $\Delta_r H^\circ_{298}$.

2(15). Using the value of $\Delta_r H^\circ_{298}$ from Question 1 and the thermal enthalpy data given at 298 K, calculate $\Delta_r H^\circ_0$.

Using $\Delta_r H^\circ_0$ and the thermal enthalpy data given at 1000 K, calculate $\Delta_r H^\circ_{1000}$.

The release/gain of energy is one of the driving forces for the spontaneity of a reaction. Is the energy change for this reaction more or is it less favorable at 1000 K than at 298 K? _____

3(20). Using the third law entropy data at 298 K, calculate $\Delta_r S^\circ_{298}$.

Using $\Delta_r C_p^\circ$ expressed in terms of the Shomate equation $C_p^\circ = A + BT + CT^2 + DT^3 + ET^{-2}$, derive the equation for $\Delta_r S^\circ_T$ expressed in terms of $\Delta_r S^\circ_{298}$, T , and the Shomate constants.

Using the Shomate constants, calculate $\Delta_r S^\circ_{1000}$.

Increase or decrease of entropy is one of the driving forces for the spontaneity of a reaction. Is this entropy change for the reaction more or is it less favorable at 1000 K than at 298 K? _____

4(10). Using $\Delta_r G^\circ_{298}$ data, calculate $\Delta_r G^\circ_{298}$.

Using the value of $\Delta_r H^\circ_{1000}$ from Question 2 and $\Delta_r S^\circ_{1000}$ from Question 3, calculate $\Delta_r G^\circ_{1000}$.

Is the reaction more or is it less spontaneous at 1000 K than at 298 K? _____

5(15). A molar sample of Ne acting as an ideal gas is compressed isothermally and isobarically from 1.00 bar to 10.00 bar at 25 °C using an external pressure of 500.0 bar. Calculate $\Delta S(\text{system})$.

Calculate $\Delta S(\text{surroundings})$.

Calculate $\Delta S(\text{universe})$.

6(25). Heat capacity data are known for the three solid forms, the liquid phase, and the gaseous phase of molecular oxygen from 11.75 K to 298 K. The values of ΔH for the various phase transformations are also known. Explain fully how S°_{298} can be determined from these data.

Using the electronic, vibrational, and rotational spectroscopic data, calculate S_{298}° for $O_2(g)$.

Does the statistical mechanical value of S_{298}° differ from the thermodynamic value by the factor of $R \ln 2$? _____