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Computational Chemistry CHEM 413/ENCH 413

1. Essentials Of Computational Chemistry: Theories

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What Is So Important About The Variables C_p , C_v , P , V ,

T ? As A Sample Application, We Can Assume The Ideal Gas Equation Of State. $V = RT /P \Rightarrow (\partial V / \partial T)_P = R/P .$
 Substitution $\Rightarrow \Delta S = C_P \ln(T_2/T_1) - R \ln(P_2/P_1)$
 Applying $\Delta S = 0 \Rightarrow \ln(T_2/T_1) = R/ C_p \ln(P_2/P_1) \Rightarrow (T_2/T_1) = (P_2/P_1)^{(C_P - C_V)/C_P}$ Mar 4th, 2024

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