

AS – 5680 High Temperature Gas Dynamics
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Supplementary Exercise – 3
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1. Derive expressions for H, G and S for each mode of energy (trans, rot, vib) of a molecule.
2. Plot C_v/k vs T/θ for vibration mode and rotation mode. Note what the value of C_v/k is at $T=\theta$. And find T/θ above which error of C_v/k from equipartition law is less than 1%. What is the change in the formula due to symmetry factor?
 (b) Do the same for electronic level assuming only one excited level exists. Take $Q = g_0 + g_1 \exp(-\theta_{elec1}/T)$
3. Find H and S as a function of T in the range of 300 to 6000K for CO₂ molecule (data given below) and compare with JANAF tables. Assume that there is no dissociation.

Species	Theta_r [K]	Theta_v [K]	Q_el	Heat of formation at 298K [kJ/mol]
CO ₂	0.56	1915 961 961 3383	$1 + \exp(-90000/T)$	-393.522

4. Refer to the problem number 3. Find out at what temperatures there is change in the C_p of the gas. Try explaining all the changes in C_p of the gas.