STATISTICAL MECHANICS
Ensemble Homework Problems

1) Consider an ensemble of just 3 systems A, B, and C with three energy states, E_1, E_2, and E_3 available to each system.

	E_1	E_2	E_3	$\Omega(n)$	P_{dist}
Dist 1					
Dist 2					
Dist 3					
Dist 4					
Dist 5					
Dist 6					
Dist 7					
Dist 8					
Dist 9					
Dist 10					
P_j					

Here $\Omega(n)$ = degeneracy of the n^{th} distribution, and P_{dist} its probability in the ensemble. The numbers you are to put into the boxes are the occupation numbers eg, 2,1,0 etc. assuming **no** restrictions on E_{total}. Make sure you can write out all 27 possible ensemble states in terms of A, B and C corresponding to the 10 possible distributions. Then, calculate the total degeneracy, $\Omega_T(n)$**,** of each distribution and the total degeneracy of the entire ensemble thus verifying the formula:

$$\sum_{all\,distributions} \frac{N_T!}{\prod_{n_i=1}^{s} n_i!} = s^{N_T}$$

where the only restriction is: $\sum_{all\ distributions} n_i = N_T$

and s = number of energy states available to each system (3 systems and 3 energy states in this case). How would you rationalize the right hand side of this formula? Now compute the probability of each ensemble energy state P_1, P_2 and P_3 using:

$$P_j = \frac{1}{N_T} \frac{\sum_{\{n\}} \Omega(n) n_j(n)}{\sum_{\{n\}} \Omega(n)}$$

The next problem does assume a restriction on E_T as well as N_T.

2) A little more realistic problem uses the constraints on N_T and E_T. So let $E_1 = E_2 = 2$ and $E_3 = E_4 = 3$ and $E_5 = 4$ where $E_{total} = 12$ and $N_T = 4$. Again, write out all possible occupation numbers for the ensemble distributions. Then calculate the degeneracy for each distribution as before. Finally, calculate the probabilities of all five system states. Using these results, compute the average energy of a system picked at random from the ensemble and confirm that it equals E_T/N_T.

	E_1=2	**E_2=2**	**E_3=3**	**E_4=3**	**E_5=4**	$\Omega(n)$	**P_{dist}**
Dist 1							
Dist 2							
Dist 3							
Dist 4							
Dist 5							
Dist 6							
Dist 7							
Dist 8							
Dist 9							
Dist 10							
Dist 11							
Dist 12							
Dist 13							
Dist 14							
Etc. ??							
P_j							

Using the table compute:

$$\bar{E} = \sum_{states} P_i E_i =$$

$$\bar{E} = E_T / N_T =$$

Question: what would the total degeneracy, Ω_T, of the ensemble be *if all of the E_i's were the same*? _____________

What would the average energy be in this case? _____________

DW McClure, Emeritus Professor of Chemistry/Physics
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