Problem set 2

$B = 20.56\ cm^{-1}$ for HF.

kT at 300K = ~$200 cm^{-1}$

kT at 600K = ~$400\ cm^{-1}$

kT at 50K = ~$35 cm^{-1}$

Table showing the calculations for populations at 300K

J	Energy (E_J) (in units of B)	Energy (E_J) (in units of cm^{-1})	Value of E_J/kT **(at 300K)**	Value of $e^{-(E_J/kT)}$	Value of 2J+1	Value of $(2J+1)\ e^{-(E_J/kT)}$
0	0	0	1	1	1	1
1	2B	41.1	0.206	0.814	3	2.4
2	6B	123.4	0.617	0.540	5	**2.7**
3	12B	246.7	1.234	0.291	7	2.0
4	20B	411.2	2.056	0.128	9	1.2
5	30B	616.8	3.084	0.046	11	0.5
6	42B	863.5	4.318	0.013	13	0.2
7	56B	1151.4	5.757	0.003	15	0.05
8	72B	1480.3	7.402	0.0006	17	0.01
9	90B	1850.4	9.252	9.6×10^{-5}	19	0.002

J_{max} (from formula: $\{[kT/2hcB]^{1/2} - 0.5\}$) at 300 K = 2

Agrees with the table

Table showing the calculations for populations at 600K

J	Energy (E_J) (in units of B)	Energy (E_J) (in units of cm^{-1})	Value of E_J/kT **(at 600K)**	Value of $e^{-(E_J/kT)}$	Value of 2J+1	Value of $(2J+1)\, e^{-(E_J/kT)}$
0	0	0	1	1	1	1
1	2B	41.1	0.103	0.903	3	2.7
2	6B	123.4	0.309	0.735	5	3.7
3	12B	246.7	0.617	0.540	7	**3.8**
4	20B	411.2	1.036	0.355	9	3.2
5	30B	616.8	1.542	0.214	11	2.4
6	42B	863.5	2.159	0.115	13	1.5
7	56B	1151.4	2.879	0.056	15	0.8
8	72B	1480.3	3.701	0.025	17	0.4
9	90B	1850.4	4.626	0.010	19	0.19

J_{max} (from formula: $\{[kT/2hcB]^{1/2} - 0.5\}$) at 600 K = 3

Agrees with the table

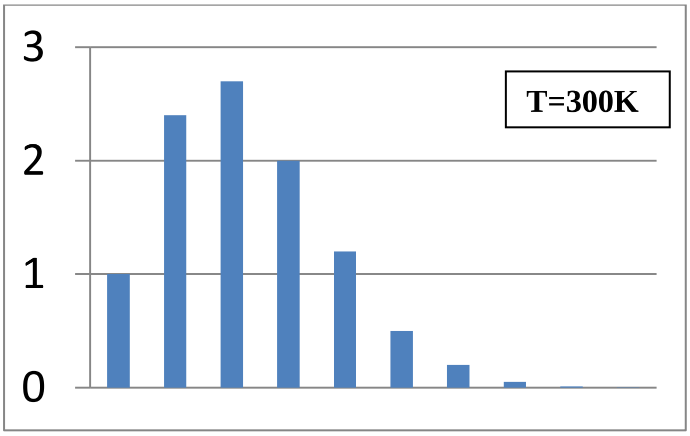
Table showing the calculations for populations at 50K

J	Energy (E_J) (in units of B)	Energy (E_J) (in units of cm^{-1})	Value of E_J/kT **(at 50K)**	Value of $e^{-(E_J/kT)}$	Value of 2J+1	Value of $(2J+1)\, e^{-(E_J/kT)}$
0	0	0	1	1	1	**1**
1	2B	41.1	1.175	0.309	3	0.9
2	6B	123.4	3.526	0.029	5	0.1
3	12B	246.7	7.049	0.0008	7	0.006
4	20B	411.2	11.749	7.9×10^{-6}	9	~0
5	30B	616.8	17.622		11	
6	42B	863.5	24.671		13	
7	56B	1151.4	32.900		15	
8	72B	1480.3			17	
9	90B	1850.4			19	

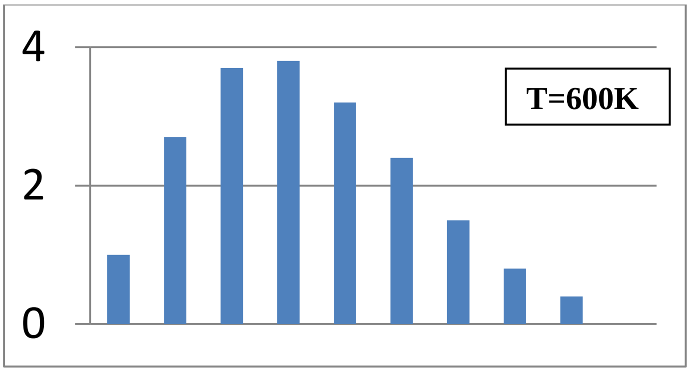
J_{max} (from formula: $\{[kT/2hcB]^{1/2} - 0.5\}$) at 300 K = 1

Agrees with the table

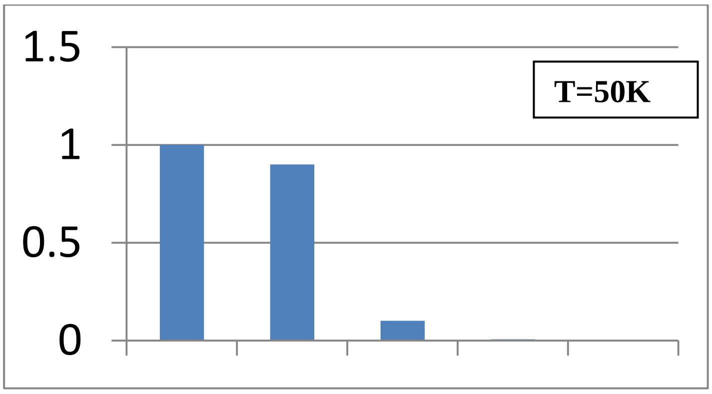
<u>Histogram showing population distribution for various J levels at various temperatures</u>



J 0 1 2 3 4 5 6 7 8



J 0 1 2 3 4 5 6 7 8



J 0 1 2 3

Note how the population shifts to higher J values with increase in temperature

Repeat the exercise for the HI example given in the next problem, to understand the effect of B values on the population.