Problem Set 10 Answers

$H =$

	ααα	ααβ	αβα	βαα	αββ	βαβ	ββα	βββ
ααα	$-\frac{1}{2}[\nu_1+\nu_2+\nu_3]+\frac{1}{4}[J_{12}+J_{13}+J_{23}]$							
ααβ		$-\frac{1}{2}[\nu_1+\nu_2-\nu_3]+\frac{1}{4}[J_{12}-J_{13}-J_{23}]$	$\frac{1}{2}J_{23}$	$\frac{1}{2}J_{13}$				
αβα		$\frac{1}{2}J_{23}$	$-\frac{1}{2}[\nu_1-\nu_2+\nu_3]+\frac{1}{4}[-J_{12}+J_{13}-J_{23}]$	$\frac{1}{2}J_{12}$				
βαα		$\frac{1}{2}J_{13}$	$\frac{1}{2}J_{12}$	$-\frac{1}{2}[-\nu_1+\nu_2+\nu_3]+\frac{1}{4}[-J_{12}-J_{13}+J_{23}]$				
αββ					$-\frac{1}{2}[\nu_1-\nu_2-\nu_3]+\frac{1}{4}[-J_{12}-J_{13}+J_{23}]$	$\frac{1}{2}J_{12}$	$\frac{1}{2}J_{13}$	
βαβ					$\frac{1}{2}J_{12}$	$-\frac{1}{2}[-\nu_1+\nu_2-\nu_3]+\frac{1}{4}[-J_{12}+J_{13}-J_{23}]$	$\frac{1}{2}J_{23}$	
ββα					$\frac{1}{2}J_{13}$	$\frac{1}{2}J_{23}$	$-\frac{1}{2}[-\nu_1-\nu_2+\nu_3]+\frac{1}{4}[J_{12}-J_{13}-J_{23}]$	
βββ								$-\frac{1}{2}[-\nu_1-\nu_2-\nu_3]+\frac{1}{4}[J_{12}+J_{13}+J_{23}]$

H =

	ααα	ααβ	αβα	βαα	αββ	βαβ	ββα	βββ
ααα	-90×10^{6} -44.275							
ααβ		-30×10^{6} +4.875	- 0.65	+3.7				
αβα		- 0.65	-30×10^{6} - 4.225	+7.4				
βαα		+3.7	+7.4	-30×10^{6} - 55.375				
αββ					$+30\times10^{6}$ +43.625	+7.4	+3.7	
βαβ					+7.4	$+30\times10^{6}$ +1.175	- 0.65	
ββα					+3.7	- 0.65	$+30\times10^{6}$ - 0.525	
βββ								$+90\times10^{6}$ +54.725

H =

	Ψ_1	Ψ_4	Ψ_3	Ψ_2	Ψ_7	Ψ_6	Ψ_5	Ψ_8
Ψ_1	-90×10^{6} -44.275							
Ψ_4		-30×10^{6} +5.106						
Ψ_3			-30×10^{6} - 3.1778					
Ψ_2				-30×10^{6} - 56.653				
Ψ_7					$+30\times10^{6}$ $^{+}$45.1525			
Ψ_6						$+30\times10^{6}$ +0.8668		
Ψ_5							$+30\times10^{6}$ - 1.7444	
Ψ_8								$+90\times10^{6}$ +54.725

C =

	Ψ_1	Ψ_4	Ψ_3	Ψ_2	Ψ_7	Ψ_6	Ψ_5	Ψ_8
ααα	1.0							
ααβ		0.0582	0.1412	0.9883				
αβα		-0.0234	0.9899	-0.1401				
βαα		0.9980	0.0149	-0.0609				
αββ					0.0773	-0.5996	0.7965	
βαβ					0.1643	0.7957	0.5830	
ββα					0.9834	-0.0858	-0.1600	
βββ								1.0

Eigenstate	Eigenfunction	Eigenvalues
Ψ_1	ααα	$E_1 = -90\times10^6 - 44.275$
Ψ_2	$0.9883\alpha\alpha\beta - 0.1401\alpha\beta\alpha - 0.0609\beta\alpha\alpha$	$E_2 = -30\times10^6 - 56.653$
Ψ_3	$0.1412\alpha\alpha\beta + 0.9899\alpha\beta\alpha + 0.0149\beta\alpha\alpha$	$E_3 = -30\times10^6 - 3.1778$
Ψ_4	$0.0582\alpha\alpha\beta - 0.0234\alpha\beta\alpha + 0.9980\beta\alpha\alpha$	$E_4 = -30\times10^6 + 5.106$
Ψ_5	$0.7965\alpha\beta\beta + 0.5830\beta\alpha\beta - 0.1600\beta\beta\alpha$	$E_5 = +30\times10^6 - 1.7444$
Ψ_6	$-0.5996\alpha\beta\beta + 0.7957\beta\alpha\beta - 0.0858\beta\beta\alpha$	$E_6 = +30\times10^6 + 0.8668$
Ψ_7	$0.0773\alpha\beta\beta + 0.1643\beta\alpha\beta + 0.9834\beta\beta\alpha$	$E_7 = +30\times10^6 + 45.1525$
Ψ_8	βββ	$E_8 = +90\times10^6 + 54.725$

$F_x =$

	ααα	ααβ	αβα	βαα	αββ	βαβ	ββα	βββ
ααα		½	½	½				
ααβ	½				½	½	0	
αβα	½				½	0	½	
βαα	½				0	½	½	
αββ		½	½	0				
βαβ		½	0	½				
ββα		0	½	½				
βββ					½	½	½	

$F_x =$

	Ψ_1	Ψ_2	Ψ_3	Ψ_4	Ψ_5	Ψ_6	Ψ_7	Ψ_8
Ψ_1		0.39365	0.5729	0.51643				
Ψ_2	0.39365				0.6242	0.1233	0.010	
Ψ_3	0.5729				0.4156	0.3201	0.55068	
Ψ_4	0.51643				0.24377	0.3679	0.5674	
Ψ_5		0.6242	0.4156	0.24377				0.6097
Ψ_6		0.1233	0.3201	0.3679				0.055
Ψ_7		0.010	0.55068	0.5674				0.6125
Ψ_8					0.6097	0.055	0.6125	

Transition	Frequency, Hz = E_t-E_s = 60×10^6 and	Intensity $\{ [\mathbf{F_x}]_{st} \}^2$
E_2-E_1	-12.378	0.155
E_3-E_1	+41.09	0.328
E_4-E_1	+49.38	0.267
E_8-E_5	+56.47	0.372
E_8-E_6	+53.86	0.003
E_8-E_7	+9.575	0.375
E_7-E_4	+40.05	0.322
E_7-E_3	+48.33	0.303
E_7-E_2	+101.80	0.000 1
E_6-E_4	-4.24	0.135
E_6-E_3	+4.04	0.102
E_6-E_2	+57.52	0.015
E_5-E_4	-6.85	0.059
E_5-E_3	+1.43	0.173
E_5-E_2	+54.91	0.390

Ordered according to frequency:

Transition	Frequency, Hz = E_t-E_s = 60×10^6 and	Intensity $\{ [\mathbf{F_x}]_{st} \}^2$
E_7-E_2	+101.80	0.000 1
E_6-E_2	+57.52	0.015
E_8-E_5	+56.47	0.372
E_5-E_2	+54.91	0.390
E_8-E_6	+53.86	0.003
E_4-E_1	+49.38	0.267
E_7-E_3	+48.33	0.303
E_3-E_1	+41.09	0.328
E_7-E_4	+40.05	0.322
E_8-E_7	+9.575	0.375
E_6-E_3	+4.04	0.102
E_5-E_3	+1.43	0.173
E_6-E_4	-4.24	0.135
E_5-E_4	-6.85	0.059
E_2-E_1	-12.378	0.155