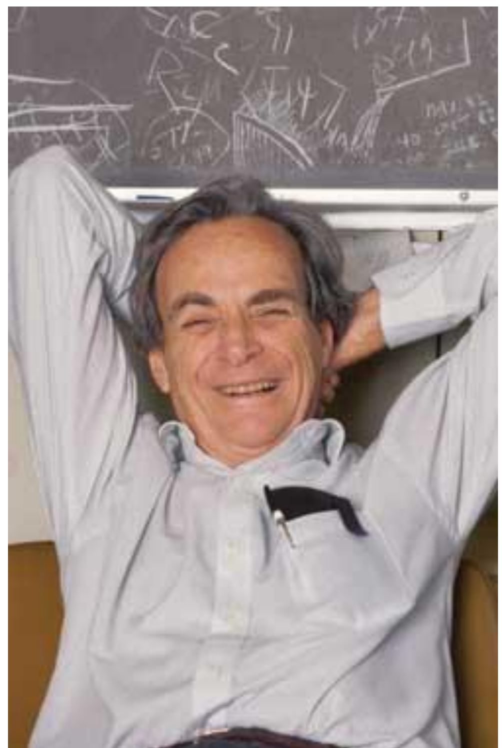
Can we build individual molecules atom by atom?

Lecture 2

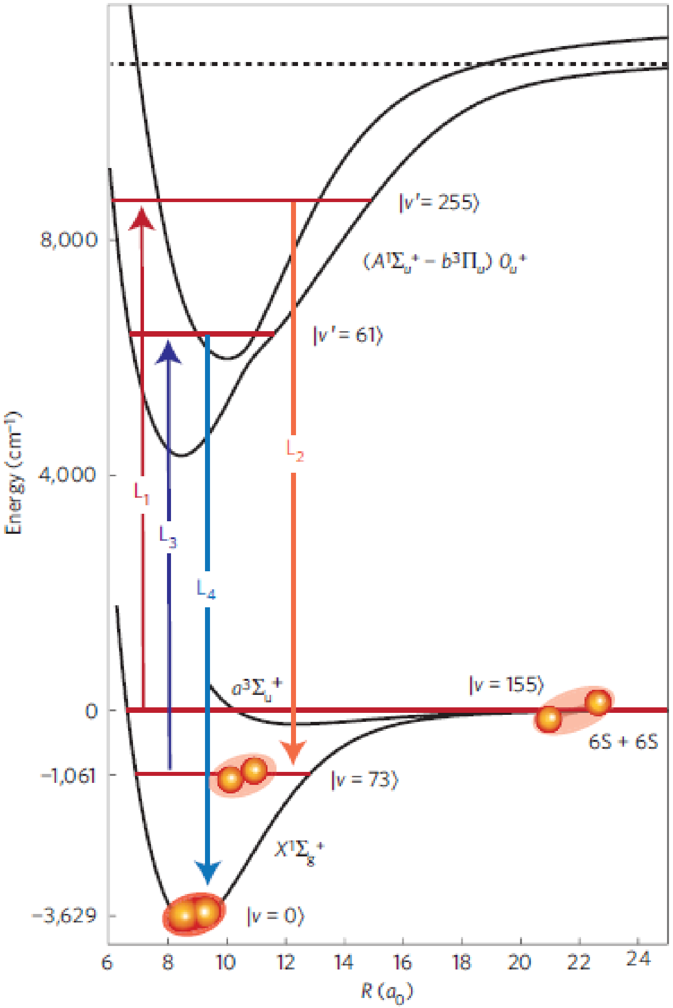


Yesterday we

- Talked about two-level atoms in light
- Optical trapping of atoms
- Laser cooling of atoms
- Dave explained how to cool all the way to the ground state (Same thing works for a single neutral atom in an optical micro-trap)
- Found that the students do not participate much in the lectures
- This provide the initialisation step of our atoms.

What is the difference between molecular physics and chemistry?

Basic molecular physics



The Hamiltonian

$$T_e = \sum_{j=1}^{N} -\frac{\hbar^2}{2m_e}\nabla^2_{\mathbf{r}_j}$$

$$T_N = -\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{R}} = -\frac{\hbar^2}{2\mu}\left(\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right) - \frac{\mathbf{N}^2}{\hbar^2 R^2}\right)$$

$$\mathbf{N}^2 = -\hbar^2\left(\frac{1}{\sin\left(\Theta\right)}\frac{\partial}{\partial \Theta}\left(\sin\left(\Theta\right)\frac{\partial}{\partial \Theta}\right) + \frac{1}{\sin^2\left(\Theta\right)}\frac{\partial^2}{\partial \Phi^2}\right)$$

$$V\left(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2 \ldots\right) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 R} - \sum_{j=1}^{N}\frac{Z_1 e^2}{4\pi\varepsilon_0\left|\mathbf{r}_j - \mathbf{R}_1\right|} - \sum_{j=1}^{N}\frac{Z_2 e^2}{4\pi\varepsilon_0\left|\mathbf{r}_j - \mathbf{R}_2\right|} + \sum_{i>j}\frac{e^2}{4\pi\varepsilon_0\left|\mathbf{r}_j - \mathbf{r}_i\right|}$$

Nuclear equation

$$\sum_q \left\langle \phi_s \middle| -\frac{\hbar^2}{2\mu}\left(\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right) - \frac{\mathbf{N}^2}{R^2}\right) \middle| \phi_q \right\rangle F_s\left(\mathbf{R}\right) + \left(E_s\left(R\right) - E\right) F_s\left(\mathbf{R}\right) = 0$$

Separate S. E. Equations

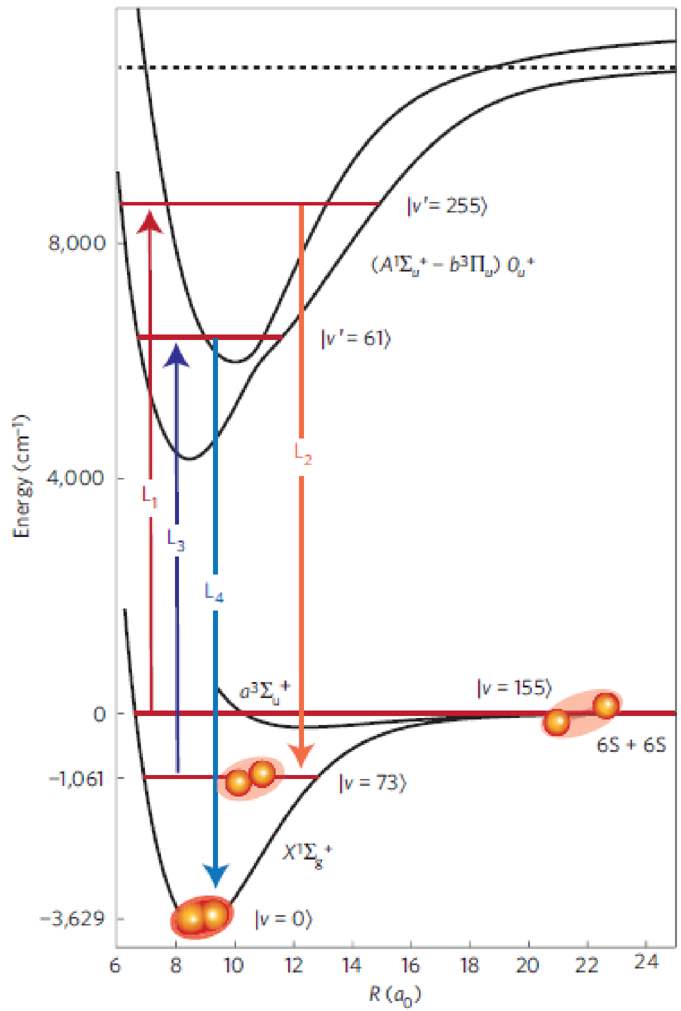
Nuclear motion:

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right)+\frac{\langle\Phi_s\left|\mathbf{N}^2\right|\Phi_s\rangle}{2\mu R^2}+E_s\left(R\right)\right)F_s\left(\mathbf{R}\right)=EF_s\left(\mathbf{R}\right)$$

Electrons. For all R solve:

$$\left(T_e+V\right)\Phi_q=E_q\left(R\right)\Phi_q$$

Basic molecular physics



We start from

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right)+\frac{\langle\Phi_s\,|\mathbf{N}^2|\,\Phi_s\rangle}{2\mu R^2}+E_s\,(R)\right)F_s\,(\mathbf{R})=EF_s\,(\mathbf{R})$$

A bit of algebra

We arrive at

$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right)-\frac{K\left(K+1\right)}{R^2}\right)F_s\left(\mathbf{R}\right)\left(E_s'\left(R\right)-E\right)F_s\left(\mathbf{R}\right)=0$$

$$\left(-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR^2}-\frac{K\left(K+1\right)}{R^2}\right)+E_s'\left(R\right)-E_{s,\nu,K}\right)\mathcal{F}_{s,\nu,K}\left(R\right)=0$$

Two conclusions

- Di-atomic molecules are indeed “physics”
- But the physics is very rich

Dipole operator for molecule

$$\mathbf{D} = e\left(\sum Z_i \mathbf{R}_i - \sum \mathbf{r}_j\right)$$

Selection rules for transitions that do not change electronic state:

- Hetero nuclear:

$$\Delta K = 0, \pm 1$$

$$\Delta M_K = 0, \pm 1$$

$$\Delta \nu = \pm 1$$

- Homo nuclear: No allowed transitions

Franck-Condon Principle
Different electronic states

$$\langle \Psi_b \left| \mathbf{D} \right| \Psi_a \rangle = \left\langle \Psi_b \middle| e \left(\sum Z_i \mathbf{R}_i - \sum \mathbf{r}_j \right) \middle| \Psi_a \right\rangle \approx \left\langle \Phi_b \middle| -e \sum \mathbf{r}_j \middle| \Phi_a \right\rangle \langle \nu_b | \nu_a \rangle$$

Formation of Ultracold Polar Molecules in the Rovibrational Ground State

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