1 Atomic Units

a. Speed of light

Solution: To find the speed of light in atomic units it would be useful to remember the *fine structure constant* defined as

$$\frac{e^2}{4\pi\epsilon_0\hbar c} = \frac{1}{137}, \tag{1}$$

but since $e = \hbar = 1/4\pi\epsilon_0 = 1$ eq. 1 turns into

$$\frac{1}{c} = \frac{1}{137},$$
$$\Rightarrow \boxed{c = 137}. \tag{2}$$

b. Bohr's Magneton

Solution: Bohr magneton is defined as

$$\mu_B = \frac{e\hbar}{2m_e}, \tag{3}$$

now, from the fact that $e = \hbar = m_e = 1$ we can deduce the numerical value

$$\mu_B = \frac{e\hbar}{2m_e} = \boxed{\frac{1}{2}}. \tag{4}$$

In both questions we went from SI units to atomic ones.

2 Magnetic Moment

a. Calculate the magnetic moment

Solution: For this problem first it might be useful to remember the definition of the $\hat{L}$ operator

$$\hat{L} = \frac{\hbar}{i}\vec{r} \times \nabla \tag{5}$$

Now let's begin our calculations

$$\begin{aligned}
\vec{m} &= \frac{1}{2}\int \vec{r} \times \vec{j}_e d^3r = \frac{1}{2}\int \vec{r} \times \left(\frac{-e\hbar}{2im_e}\right)\left(\psi^*_{n,l,m}\nabla\psi_{n,l,m} - \psi_{n,l,m}\nabla\psi^*_{n,l,m}\right) d^3r, \\
&= \frac{1}{2}\int \left(\frac{-e\hbar}{2im_e}\right)\psi^*_{n,l,m}\vec{r} \times \nabla\psi_{n,l,m} - \left(\frac{-e\hbar}{2im_e}\right)\psi_{n,l,m}\vec{r} \times \nabla\psi^*_{n,l,m} d^3r, \\
&= \frac{1}{2}\left(\frac{-e}{2m_e}\right)\int \psi^*_{n,l,m}\hat{L}\psi_{n,l,m} - \psi_{n,l,m}\hat{L}\psi^*_{n,l,m} d^3r, \qquad \text{using eq. 5}, \\
&= \frac{1}{2}\left(\frac{-e}{2m_e}\right) 2\left\langle \psi_{n,l,m} \middle| \hat{L} \middle| \psi_{n,l,m} \right\rangle, \\
&= \frac{-e}{2m_e}\left\langle \psi_{n,l,m} \middle| \hat{L} \middle| \psi_{n,l,m} \right\rangle,
\end{aligned}$$

$$= \frac{-e\hbar}{2\hbar m_e} \left\langle \psi_{n,l,m} \middle| \hat{L} \middle| \psi_{n,l,m} \right\rangle,$$

and finally

$$= \boxed{\frac{-\mu_B}{\hbar} \left\langle \psi_{n,l,m} \middle| \hat{L} \middle| \psi_{n,l,m} \right\rangle,} \quad \text{using eq. 7} \tag{6}$$

where in the last step we used the definition of Bohr magneton

$$\mu_B = \frac{e\hbar}{2m_e}. \tag{7}$$

So as we can see there's a direct connection between $\vec{m}$ and the expectation value of the angular momentum operator.

b. z-components

Solution: If we are only interested in the z component of the magnetic moment then from eq. 6 we can isolate the z term of $\hat{L}$, and the resulting equation will be

$$m_z = -\frac{\mu_B}{\hbar} \left\langle \psi_{n,l,m} \middle| \hat{L}_z \middle| \psi_{n,l,m} \right\rangle, \tag{8}$$

if we remember, the eigenvalue equation for $\hat{L}_z$ is

$$\hat{L}_z \left|\psi_{n,l,m}\right\rangle = \hbar m \left|\psi_{n,l,m}\right\rangle. \tag{9}$$

Pluging eq. 9 into eq. 8 we get

$$\begin{aligned} m_z &= -\frac{\mu_B}{\hbar} \left\langle \psi_{n,l,m} \middle| \hat{L}_z \middle| \psi_{n,l,m} \right\rangle, \\ &= -\frac{\mu_B}{\hbar} \left\langle \psi_{n,l,m} \middle| \hbar m \middle| \psi_{n,l,m} \right\rangle, \\ &= -\mu_B m \cancelto{1}{\langle \psi_{n,l,m} | \psi_{n,l,m} \rangle}, \\ &= -\mu_B m. \end{aligned}$$

Therefore

$$[m_{n,l,m}]_z = -\mu_B m, \tag{10}$$

and we can use this to calculate what we need.

- $[m_{100}]_z = -\mu_B(m) = -\mu_B(0) = \boxed{0}$
- $[m_{200}]_z = \boxed{0}$, for the same reason as above
- $[m_{21-1}]_z = -\mu_B(-1) = \boxed{\mu_B}$
- $[m_{210}]_z = -\mu_B(0) = \boxed{0}$
- $[m_{211}]_z = -\mu_B(1) = \boxed{-\mu_B}$
- $[m_{532}]_z = -\mu_B(2) = \boxed{-2\mu_B}$

3 Charge States

a. Formal Charge

Solution: In the case of the first compuond we have $KCrF_3$, the charges we know are

- $K = 1$.
- $F_3 = 3(-1) = -3$.

So in order to neutralize the charge we need

- $Cr = -(1-3) = -(-2) = 2.$

The next compound is $SrMnO_3$, the charges we know are

- $Sr = 2$.
- $O_3 = 3(-2) = -6$

Hence, the charge we need is

- $Mn = -(2-6) = -(-4) = 4.$

4 Atomic Radii

a. Read article

Solution: I did not read it but it's on my to-do list now ;)