HW #8 Answers

1. 

a_1' e' e' ← D_{3h}

a_1 b_1 or b_2 a_1 ← C_{2v}

↳ depending on orientation of axes

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2. The integral involves $e^{-\alpha\sqrt{x^2+y^2+z^2}}$.

$e^{-\alpha\sqrt{x^2+y^2+(z-R)^2}}$

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3. Ground state $a_{2u}^2 e_{2u}^4 \rightarrow {}^1A_{1g}$

excited states $a_{2u}^2 e_{2u}^3 e_{1g}$

So we need to consider $e_{2u} \times e_{1g}$

This tells us that there are B_{1u}, B_{2u}, and E_{1u} electronically excited states. In each case there is a singlet and a triplet spin state.

From the point group character table we see that (x, y) transform according to the E_{1u} representation and z according to the A_{2u} representation. So the ${}^1E_{2u}$ would be dipole allowed, but ${}^1B_{1u}$ and ${}^1B_{2u}$ are