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"Use definition (3.219) for the STO-1G function and the scaling relation (3.224) to show that the STO-1G overlap for an orbital exponent  $\zeta = 1.24$  at  $R = 1.4$  a. u., corresponding to result (3.229), is  $S_{12} = 0.6648$ . Use the formula in Appendix A for overlap integrals. Do not forget normalization ...

### **Szabo, A.; Ostlund, N. S. (1996). MODERN QUANTUM CHEMISTRY ...**

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Homework: Four homework assignments will be given during the semester, each of which must be turned in by 6:00 PM on the due date. In addition, we will hold one "molecular show" in which each student will present an electronic structure calculations for a given molecule.

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