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Exercise. This is the solution to exercise 1.13 in the book. Solution. If we consider matrix $U = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}$ such that $U^\dagger A U = \begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix}$. then we get $\theta = \frac{1}{2} \arctan \frac{\Delta}{a}$, or $2\theta = \arctan \frac{\Delta}{a}$, hence $\theta = \frac{1}{4} \arctan \frac{\Delta}{a}$. Therefore

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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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