

9. List all the independent 2e integrals for a minimal basis set calculation on H_2

$$u_1 = \phi_{1s}^a$$

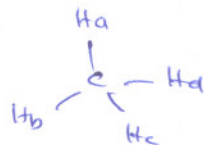
$$u_2 = \phi_{1s}^b$$

$$\text{2-centre} \begin{cases} (u_1, u_1 | u_1, u_1) \\ (u_1, u_1 | u_2, u_2) \\ (u_1, u_2 | u_1, u_2) \\ (u_1, u_2 | u_2, u_2) \end{cases}$$

Write these in expanded form.

10. For a minimal basis set calculation on CH_4 give ~~the~~ examples ~~for~~ 1-centre, 2-centre, 3-centre and 4-centre 2e integrals.

$$u_1 = \phi_{1s}^a \quad u_2 = \phi_{1s}^b \quad u_3 = \phi_{1s}^c \quad \& \quad u_4 = \phi_{1s}^d$$



$$u_5 = C(1s) \quad u_6 = C(2s) \quad u_7 = C(2p_x) \quad u_8 = C(2p_y) \quad u_9 = C(2p_z)$$

1-centre integrals: $(u_1, u_1 | u_1, u_1); (u_5, u_5 | u_5, u_5);$

$(u_5, u_6 | u_5, u_6);$ etc..

2-centre : $(u_1, u_2 | u_1, u_2); (u_1, u_6 | u_7, u_8)$ etc..

3-centre : $(u_1, u_2 | u_3, u_3); (u_6, u_5 | u_1, u_3)$ etc..

4-centre : $(u_1, u_2 | u_3, u_4); (u_1, u_2 | u_4, u_9)$ etc..

Try writing a computer program to list all the independent 2e integrals.