

Example 14. Calculate Z_{eff} for (i) 4s and (ii) 3d electron in iron atom

$$Z = (26, 1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^6, 4s^2)$$

Solution. Group configuration = $(1s^2); (2s^2, 2p^6); (3s^2, 3p^6); (3d^6); (4s^2)$

(i) For 4s electron, $S = (10 \times 1.00) + (14 \times 0.85) + (1 \times 0.35) = 22.25$

$$Z_{\text{eff}} = 26 - 22.25 = 3.75$$

(ii), In case of 3d electron, there is no contribution from outer 4s group electrons inner of 3d contribute one each

Example 15. Calculate the effective nuclear charge for

(i) an electron in 3d orbital, and

(ii) an electron in 4s orbital of chromium ($Z = 24$) with electronic configuration = $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^5, 4s^1$

Solution. Group configuration $(1s^2), (2s^2, 2p^6), (3s^2, 3p^6), (3d^5), (4s^1)$

(i) For 3d electron. There is no contribution from outer 4s. Remaining 4 electrons in 3d contribute 4×0.35 and all others contribute one each.

$$S = (18 \times 1) + (4 \times 0.35) + (4 \times 0)$$

$$= 18 + 1.40 + 0 = 19.40$$

$$Z_{\text{eff}} = 24 - 19.40 = 4.60$$

(ii) For 4s electron. There are no other electron in 4s. Consequently there is no contribution and we have $0 \times 0.35 = 0$.

Next inner shell ($n = 3$) has 13 electrons contributing 13×0.85 , others contribute each and we have

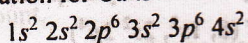
$$S = (10 \times 1) + (13 \times 0.85) + (0 \times 0.35)$$

$$= 10 + 11.45 + 0 = 21.45$$

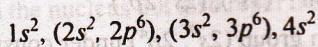
$$Z_{\text{eff}} = 24 - 21.45 = 2.55$$

Example 16. Calculate Z_{eff} for valence electrons in Ca and Br.

Solution. (a) Electronic configuration for Ca is



This can be grouped as



Screening constant of 4s electron

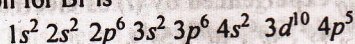
$$= (1 \times 0.35) + (8 \times 0.85) + (10 \times 1)$$

$$= 17.15$$

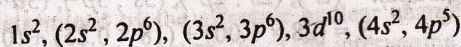
Hence

$$Z_{\text{eff}} = 20 - 17.15 = 2.85$$

(b) Electronic configuration for Br is



This can be grouped as



Screening constant of 4p electron

$$= (4 \times 0.35) + (10 \times 0.85) + (18 \times 1)$$

$$= 27.9$$

Hence

$$Z_{\text{eff}} = 35 - 27.9 = 7.1$$