Example 14. **Calculate Z_{eff} for (*i*) 4s and (*ii*) 3*d* 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,** $S = (10 \times 1.00) + (14 \times 0.85) + (1 \times 0.35) = 22.25$

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

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

Example 15. **Calculate the effective nuclear charge for**

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

$$S = (18 \times 1) + (4 \times 0.35) + (4 \times 0)$$
$$= 18 + 1.40 + 0 = 19.40$$
$$Z_{eff} = 24 - 19.40 = 4.60$$

(*ii*) **For 4*s* electron.** There are no other electron in 4*s*. 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

$$S = (10 \times 1) + (13 \times 0.85) + (0 \times 0.35)$$
$$= 10 + 11.45 + 0 = 21.45$$
$$Z_{eff} = 24 - 21.45 = 2.55$$

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

Solution. (*a*) Electronic configuration for Ca is

$$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$$

This can be grouped as

$$1s^2, (2s^2, 2p^6), (3s^2, 3p^6), 4s^2$$

Screening constant of 4*s* electron

$$= (1 \times 0.35) + (8 \times 0.85) + (10 \times 1)$$
$$= 17.15$$

Hence $Z_{eff} = 20 - 17.15 = 2.85$

(*b*) Electronic configuration for Br is

$$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$$

This can be grouped as

$$1s^2, (2s^2, 2p^6), (3s^2, 3p^6), 3d^{10}, (4s^2, 4p^5)$$

Screening constant of 4*p* electron

$$= (4 \times 0.35) + (10 \times 0.85) + (18 \times 1)$$
$$= 27.9$$

Hence $Z_{eff} = 35 - 27.9 = 7.1$