

Limitations of Aufbau concept

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In the 6th of Modern Periodic table.

6th Period →

55 Cs	56 Ba	57-71 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
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58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
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In the above Configuration of Lanthanoids gr. (i.e 57-71)

4f and 5d Orbitals are close in energy level

In case of La, the last electron does not go to 4f as predicted in Aufbau Order, but goes to 5d orbital to give it $4d^{10} 5s^2 5p^6 5d^1 6s^2$ configuration.

However, the next electron for Cerium (Z=58) is added to the '4f' orbital and the previous electron in 5d in Lanthanum also goes to '4f' orbital to give its electronic configuration... $4d^{10} 5s^2 5p^6 4f^2 5d^0 6s^2$.

(4) The electronic Configuration of Zr (Z=40)

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

(Z=40) $1s^2, 2s^2 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2 4p^6, 5s^2, 4d^2$ (According to Aufbau order)

Now Aufbau electronic Configuration of Niobium Nb (Z=41)

Nb (Z=41) $1s^2, 2s^2 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2 4p^6, 5s^2, 4d^5$ (Aufbau's Configuration)

(Z=41) $1s^2, 2s^2 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2 4p^6 5s^1 4d^4$ (Experimental Observed Configuration)

Mo (Molybdenum) (Z=42) $5s^1 4d^5$ (Both configurations due to higher stability related to half-filled configuration)

Tc (Technetium) (Z=43) $[Kr] 4d^5 5s^2$

Pd (Z=46) $[Kr] 4d^{10} 5s^0$ (Correct)
 not $[Kr] 4d^8 5s^2$ (NOT)