

## Atomic and Molecular Notation

Please note the style followed in *Physical Review A* and *Physical Review E* for atomic and molecular notation.

Elements are roman:

H, Na, Cl, P, etc.

Superscripts to elements indicate charge states:

$\text{Ca}^{2+}$  (not  $\text{Ca}^{++}$ )  
 $\text{Ca}^{2+*}$  for an excited ion

Presuperscripts and presubscripts to elements indicate atomic mass and atomic number:

${}^{125}_{53}\text{I}$

For molecular ions, superscripts and subscripts are staggered:

$\text{H}_3^+$ ,  $\text{He}_2^*$ ,  $(\text{D}_2\text{O})_n^+$

Roman numerals following elements are set in small caps with a thin space separating the element and the roman numerals:

Na I

but with a full space in a series:

Na I, II, III

Letters denoting atomic configurations are set italic, with a full space between the element and the state:

Na *3p*

(but for a transition there is a thin space between the element and the configuration):

Na *3p* – Na *3d*

Superscripts to levels indicating odd and even parity are lowercase italic “oh” and “ee”:

${}^1P_{3/2}^o$ ,  ${}^1S_{3/2}^e$

Thin spaces are inserted for clarity in the following notation for atomic and molecular levels:

$3p^3P_{1/2}$ ,  $3^2P_{3/2}$ ,  $A^3\Pi_{\mu}^+$ ,  $\text{CO } X^1\Sigma^+$ ,  $\text{He II } \alpha$

For x rays, the Greek letter is on line:

$K\alpha$ ,  $K\beta$ ,  $L\alpha$ ,  $L\beta$ ,  $\text{Cu } K\alpha$ ,  $K\alpha_1$

For spectral lines of hydrogen, the Greek letter is a subscript and roman letters indicate the series:

Balmer series:  $\text{H}_{\alpha}$ ,  $\text{H}_{\beta}$   
 Lyman series:  $\text{Ly-}\alpha$ ,  $\text{Ly-}\beta$  or  
 Lyman series:  $L_{\alpha}$ ,  $L_{\beta}$  ( $\text{Ly-}\alpha$ ,  $\text{Ly-}\beta$ ,  $\text{Lyman-}\alpha$ ,  $\text{Lyman-}\beta$  are also acceptable)

Note that italic is printed for shells, edges:

$K$  shell,  $L$  shell,  $K$ -Auger-electron emission,  $K$  edge

The author’s use of parentheses allows notation to be closed up:

${}^2S_{1/2}(F = 1)$ ,  $\text{Br}^+({}^3P_2)$ ,  $\text{Ar}^{2+}(3s^23p^4)$ ,  $(3p^5{}^2P)\text{Ar}^+$

Indicate bonds with a “bond” dash:

C — N bond  
 $\angle (\text{H} — \text{O} — \text{H}) = 70^\circ$

Protons, electrons, and neutrons are indicated with lowercase italics:

$p$ ,  $e$ , and  $n$

Nucleon is spelled out.