

## IR-3 Elements and Groups of Elements (March 04)

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### IR-3.1 NAMES AND SYMBOLS OF ATOMS

The origins of the names of some chemical elements, for example antimony, are lost in antiquity. Other elements recognised (or discovered) during the past three centuries were named according to various associations of origin, physical or chemical properties, *etc.*, and more recently to commemorate the names of eminent scientists.

In the past, some elements were given two names because two groups claimed to have discovered them. To avoid such confusion it was decided in 1947 that after the existence of a new element had been proved beyond reasonable doubt, discoverers had the right to *suggest* a name to IUPAC, but that only the Commission on Nomenclature of Inorganic Chemistry (CNIC) could make a recommendation to the IUPAC Council to make the final

decision. Names for elements up to and including element 103 do not, therefore, carry any implication regarding priority of discovery.

Under the present procedure,<sup>1</sup> claims of the discovery of a new element are first investigated by a joint IUPAC-IUPAP (International Union of Pure and Applied Physics) committee which then assigns priority. The discoverers are then invited to suggest a name to the Division of Inorganic Chemistry before a formal recommendation to the IUPAC Council is made. It is emphasised that the IUPAC-approved name for any new element carries no implication regarding priority of discovery.

The IUPAC-approved names of the atoms of atomic numbers 1-110 for use in the English language are listed in alphabetical order in Table I\*; it is desirable that the names used in other languages differ from these as little as possible. Names which are not used in English (but which provide the basis of the atomic symbol), which have entered into chemical nomenclature, or which are IUPAC-approved alternatives are noted in Table I.

For use in chemical formulae, each atom is represented by a unique symbol in upright type as shown in Table I. In addition, the symbols D and T may be used for the hydrogen isotopes of mass numbers two and three respectively (see Section IR-3.3.2).

#### IR-3.1.1 *Systematic nomenclature and symbols for new elements*

Newly discovered elements may be referred to in the scientific literature but until they have received permanent names and symbols from IUPAC, temporary designators are required. Such elements may be referred to by their atomic numbers, as in 'element 120' for example, but IUPAC has approved a systematic nomenclature and series of three-letter symbols (see Table II).<sup>2</sup>

The name is derived directly from the atomic number of the element using the following numerical roots:

|         |          |          |         |
|---------|----------|----------|---------|
| 0 = nil | 3 = tri  | 6 = hex  | 9 = enn |
| 1 = un  | 4 = quad | 7 = sept |         |
| 2 = bi  | 5 = pent | 8 = oct  |         |

The roots are put together in the order of the digits which make up the atomic number and terminated by 'ium' to spell out the name. The final 'n' of 'enn' is elided when it occurs before 'nil', and the final 'i' of 'bi' and of 'tri' when it occurs before 'ium'.

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\* Tables numbered with a Roman numeral are collected together at the end of this book.

The symbol for the element is composed of the initial letters of the numerical roots which make up the name.

*Example:*

113 = ununtrium, symbol Uut

### IR-3.2 INDICATION OF MASS, CHARGE AND ATOMIC NUMBER USING INDEXES (SUBSCRIPTS AND SUPERSSCRIPTS)

The mass, charge and atomic number of a nuclide are indicated by means of three indexes (subscripts and superscripts) placed around the symbol. The positions are occupied as follows:

|                   |               |
|-------------------|---------------|
| left upper index  | mass number   |
| left lower index  | atomic number |
| right upper index | charge        |

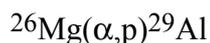
A charge placed on an atom of symbol A is indicated as  $A^{n+}$  or  $A^{n-}$ , not as  $A^{+n}$  or  $A^{-n}$ .

The right lower position of an atomic symbol is reserved for an index (subscript) indicating the number of such atoms in a formula. For example,  $S_8$  is the formula of a molecule containing eight sulfur atoms (see Section IR-3.4). For formalisms when oxidation states or charges are also shown, see Section IR-4.6.1.

*Example:*

1.  ${}^{32}_{16}\text{S}^{2+}$  represents a doubly ionized sulfur atom of atomic number 16 and mass number 32.

The nuclear reaction between  ${}^{26}_{12}\text{Mg}$  and  ${}^4_2\text{He}$  nuclei to yield  ${}^{29}_{13}\text{Al}$  and  ${}^1_1\text{H}$  nuclei is written as follows<sup>3</sup>:



For the nomenclature of isotopically modified compounds and the use of atomic symbols to indicate isotopic modification in chemical formulae see Section IR-4.5 and Chapter II-2 of Ref. 4.

### IR-3.3 ISOTOPES

### IR-3.3.1 **Isotopes of an element**

The isotopes of an element all bear the same name (but see Section IR-3.3.2) and are designated by mass numbers (see Section IR-3.2). For example, the atom of atomic number 8 and mass number 18 is named oxygen-18 and has the symbol  $^{18}\text{O}$ .

### IR-3.3.2 **Isotopes of hydrogen**

Hydrogen is an exception to the rule in Section IR-3.3.1 in that the three isotopes  $^1\text{H}$ ,  $^2\text{H}$ , and  $^3\text{H}$  can have the alternative names protium, deuterium, and tritium, respectively. The symbols D and T may be used for deuterium and tritium but  $^2\text{H}$  and  $^3\text{H}$  are preferred because D and T can disturb the alphabetical ordering in formulae (see Chapter IR-4.5). Furthermore, the combination of a muon and an electron behaves like a light isotope of hydrogen and is named muonium, symbol Mu.<sup>5</sup>

These names give rise to the names proton, deuteron, triton, and muon for the cations  $^1\text{H}^+$ ,  $^2\text{H}^+$ ,  $^3\text{H}^+$ , and  $\text{Mu}^+$ , respectively. Because the name proton is often used in contradictory senses, *i.e.* for isotopically pure  $^1\text{H}^+$  ions on the one hand, and for the naturally occurring undifferentiated isotope mixture on the other, it is recommended that the undifferentiated mixture be designated generally by the name hydron, derived from hydrogen.

## IR-3.4 ELEMENTS (or elementary substances)

### IR-3.4.1 **Name of an element of infinite or indefinite molecular formula or structure**

A sample of an element that has an undefined formula, or is a mixture of allotropes (see Section IR-3.5), bears the same name as the atom.

### IR-3.4.2 **Names of allotropes of definite molecular formula**

Allotropes of definite molecular formula are named by adding the appropriate numerical prefix (Table IV) (mono, di, tri, tetra, penta, *etc.*) to designate the number of atoms in the molecule. The prefix 'mono' is not used except when the element does not normally exist in a monoatomic state.

*Examples:*

- |    |                           |    |                                  |
|----|---------------------------|----|----------------------------------|
| 1. | H, monohydrogen           | 5. | $\text{O}_3$ , trioxygen (ozone) |
| 2. | N, mononitrogen           | 6. | $\text{P}_4$ , tetraphosphorus   |
| 3. | $\text{N}_2$ , dinitrogen | 7. | $\text{S}_8$ , octasulfur        |

## 4. Ar, argon

The prefix 'poly' may be used if the number of atoms in the molecule is large and unknown.

*Example:*

8. S<sub>n</sub>, polysulfur

## IR-3.5 ALLOTROPIC MODIFICATIONS

## IR-3.5.1 Allotropes

Allotropic modifications of an element bear the name of the atom from which they are derived, together with a descriptor to specify the modification. Common descriptors are Greek letters ( $\alpha$ ,  $\beta$ ,  $\gamma$ , *etc.*), colours and, where appropriate, mineral names (*e.g.* graphite and diamond for the well known forms of carbon). Such names should be regarded as provisional, to be used only until structures have been established, after which a rational system based on molecular formula (see Section IR-3.5.2) or crystal structure (see Section IR-3.5.3) is recommended. The well-established common names or descriptors are allowed alternatives for common structurally defined allotropes of carbon, phosphorus, sulfur, tin and iron (see Examples in Chapter IR-11, and in Section IR-3.5.3), except when they can be treated under Section IR-3.5.2. Common names will also continue to be used for amorphous modifications of an element and for those which are mixtures of closely related structures (such as graphite) in their commonly occurring forms or have an ill-defined disordered structure (such as red phosphorus) (see Section IR-3.5.4).

## IR-3.5.2 Allotropic modifications constituted of discrete molecules

Systematic names are based on the number of atoms in the molecule, indicated by a numerical prefix (see Section IR-3.4.2). If the number is large and unknown, as in long chains or large rings, the prefix 'poly' may be used. Where necessary, appropriate prefixes (Table V) may be used to indicate structure. When it is desired to specify a particular polymorphous form of a molecular element with a defined structure (such as S<sub>8</sub> in  $\alpha$ - or  $\beta$ -sulfur) the method of Section IR-3.5.3 should be used.

*Examples:*

|    | <i>Symbol</i>  | <i>Systematic name</i> | <i>Common name</i> |
|----|----------------|------------------------|--------------------|
| 1. | O <sub>2</sub> | dioxygen               | oxygen             |
| 2. | O <sub>3</sub> | trioxygen              | ozone              |

|    |                |                 |  |
|----|----------------|-----------------|--|
| 3. | P <sub>4</sub> | tetraphosphorus | white phosphorus<br>(or yellow phosphorus) |
| 4. | S <sub>6</sub> | hexasulfur      | -  |
| 5. | S <sub>8</sub> | octasulfur      | α-sulfur, β-sulfur                         |
| 6. | S <sub>n</sub> | polysulfur      | μ-sulfur (or plastic sulfur)               |

### IR-3.5.3 Crystalline allotropic modifications of an element

Crystalline allotropic modifications are polymorphs of the elements. Each can be named by adding the Pearson symbol<sup>6</sup> in parentheses after the name of the atom. This symbol defines the structure of the allotrope in terms of its Bravais lattice (crystal class and type of unit cell) and number of atoms in its unit cell (Table IR-3.1 and Chapter IR-11). Thus, iron(*cF4*) is the allotropic modification of iron ( $\gamma$ -iron) with a cubic (*c*), all-face-centred (*F*) lattice containing four atoms of iron in the unit cell. The trivial nomenclature of allotropes is discouraged.

**Table IR.3.1** Pearson symbols used for the fourteen Bravais lattices

| <i>System</i>                         | <i>Lattice symbol</i> <sup>a</sup> | <i>Pearson symbol</i> |
|---------------------------------------|------------------------------------|-----------------------|
| Triclinic                             | <i>P</i>                           | <i>aP</i>             |
| Monoclinic                            | <i>P</i>                           | <i>mP</i>             |
|                                       | <i>S</i> <sup>b</sup>              | <i>mS</i>             |
| Orthorhombic                          | <i>P</i>                           | <i>oP</i>             |
|                                       | <i>S</i>                           | <i>oS</i>             |
|                                       | <i>F</i>                           | <i>oF</i>             |
|                                       | <i>I</i>                           | <i>oI</i>             |
| Tetragonal                            | <i>P</i>                           | <i>tP</i>             |
|                                       | <i>I</i>                           | <i>tI</i>             |
| Hexagonal<br>(and trigonal <i>P</i> ) | <i>P</i>                           | <i>hP</i>             |
| Rhombohedral                          | <i>R</i>                           | <i>hR</i>             |
| Cubic                                 | <i>P</i>                           | <i>cP</i>             |
|                                       | <i>F</i>                           | <i>cF</i>             |
|                                       | <i>I</i>                           | <i>cI</i>             |

<sup>a</sup> *P*, *S*, *F*, *I*, and *R* are primitive, one-face-centred, all-face-centred, body-centred and rhombohedral lattices, respectively. <sup>b</sup> Second setting, *y*-axis unique.

In a few cases, the Pearson symbol fails to differentiate between two crystalline allotropes of the element. In such an event the space group is added to the parentheses. Thus, for example, the two forms of Se,  $\alpha$ -selenium and  $\beta$ -selenium, both  $\text{Se}_n$ , are distinguished by the symbols (*mP32*, *P2<sub>1</sub>/*n**) and (*mP32*, *P2<sub>1</sub>/*a**), respectively. Alternatively, a notation involving compound type may be useful (see Chapter IR-11).

*Examples:*

|     | <i>Symbol</i>   | <i>Systematic name</i>   | <i>Common name</i>          |
|-----|-----------------|--------------------------|-----------------------------|
| 1.  | $\text{P}_n$    | phosphorus( <i>oC8</i> ) | black phosphorus            |
| 2.  | $\text{C}_n$    | carbon( <i>cF8</i> )     | diamond                     |
| 3.  | $\text{C}_n$    | carbon( <i>hP4</i> )     | graphite (common form)      |
| 4.  | $\text{C}_n$    | carbon( <i>hR6</i> )     | graphite (less common form) |
| 5.  | $\text{Fe}_n$   | iron( <i>cI2</i> )       | $\alpha$ -iron              |
| 6.  | $\text{Fe}_n$   | iron( <i>cF4</i> )       | $\gamma$ -iron              |
| 7.  | $\text{Sn}_n$   | tin( <i>cF8</i> )        | $\alpha$ - or grey tin      |
| 8.  | $\text{Sn}_n$   | tin( <i>tI4</i> )        | $\beta$ - or white tin      |
| 9.  | $\text{Mn}_n$   | manganese( <i>cI58</i> ) | $\alpha$ -manganese         |
| 10. | $\text{Mn}_n$   | manganese( <i>cP20</i> ) | $\beta$ -manganese          |
| 11. | $\text{Mn}_n$   | manganese( <i>cF4</i> )  | $\gamma$ -manganese         |
| 12. | $\text{Mn}_n$   | manganese( <i>cI2</i> )  | $\delta$ -manganese         |
| 13. | $\text{S}_6$    | sulfur( <i>hR18</i> )    | -                           |
| 14. | $\text{S}_{20}$ | sulfur( <i>oP80</i> )    | -                           |

#### IR-3.5.4 Solid amorphous modifications and commonly recognized allotropes of indefinite structure

Solid amorphous modifications and commonly recognized allotropes of indefinite structure are distinguished by customary descriptors such as a Greek letter, names based on physical properties, or mineral names (see Examples in Section IR-3.5.3).

*Examples:*

|    |              |  |
|----|--------------|--|
| 1. | $\text{C}_n$ | amorphous carbon   |
| 2. | $\text{C}_n$ | graphitic carbon (carbon in the form of graphite, irrespective of structural defects)                            |
| 3. | $\text{P}_n$ | red phosphorus [a disordered structure containing parts of phosphorus( <i>oC8</i> ) and parts of tetrphosphorus] |

4.  $As_n$  amorphous arsenic

## IR-3.6 GROUPS OF ELEMENTS

IR-3.6.1 **Groups of elements in the Periodic Table and their subdivisions**

The groups of elements in the Periodic Table are numbered from 1 to 18. The elements (except hydrogen) of groups 1, 2, 13, 14, 15, 16, 17 and 18 are designated as Main Group elements and, except in group 18, the first two elements of each Main Group are termed Typical Elements. The elements of groups 3-11 are Transition Elements. Optionally the letters s, p, d and f may be used to distinguish different blocks of elements. If appropriate for a particular purpose, the various groups may be named from the first element in each, for example elements of the boron group (B, Al, Ga, In, Tl), elements of the titanium group (Ti, Zr, Hf, Rf), *etc.*

IR-3.6.2 **Collective names of groups of like elements**

The following collective names for groups of atoms are IUPAC-approved: alkali metals (Li, Na, K, Rb, Cs, Fr), alkaline earth metals (Be, Mg, Ca, Sr, Ba, Ra), pnictogens (N, P, As, Sb, Bi), chalcogens (O, S, Se, Te, Po), halogens (F, Cl, Br, I, At), noble gases (He, Ne, Ar, Kr, Xe, Rn), lanthanoids (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu), rare earth metals (Sc, Y and the lanthanoids), and actinoids (Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr).

The generic terms pnictide, chalcogenide, and halogenide (or halide) are used in naming compounds of the pnictogens, chalcogens, and halogens.

Although lanthanoid means 'like lanthanum' and so should not include lanthanum, lanthanum has become included by common usage. Similarly, actinoid. The ending 'ide' normally indicates a negative ion, and therefore lanthanoid and actinoid are preferred to lanthanide and actinide. However, lanthanide and actinide are still allowed owing to wide current use.

A transition element is an element whose atom has an incomplete d-sub-shell, or which gives rise to a cation or cations with an incomplete d-sub-shell. The First Transition Series of elements is Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Cu. The Second and Third Transition Series are similarly derived: these include the lanthanoids and actinoids respectively. The latter are designated inner (or f) transition elements of their respective Periods in the Periodic Table.

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6. W.B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, Vol. 2, Pergamon Press, Oxford, 1967, pp. 1,2. For tabulated lattice parameters and data on elemental metals and semi-metals, see pp. 79-91. See also, P. Villars and L.D. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, Vols. 1-3, American Society for Metals, Metals Park, Ohio, USA, 1985.