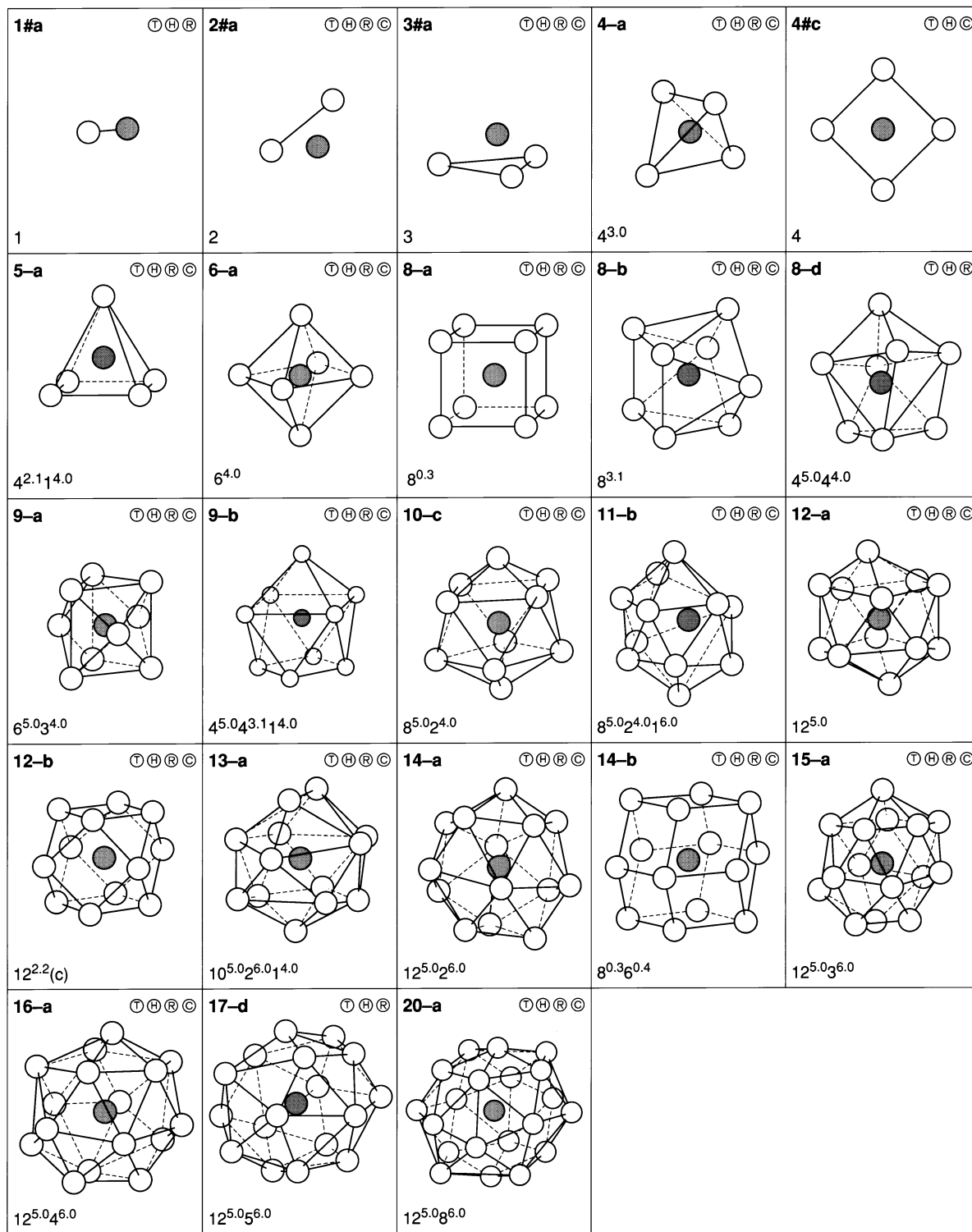


## 9. BASIC STRUCTURAL FEATURES

belonging to the cubic, rhombohedral, hexagonal, and tetragonal crystal systems (Daams & Villars, 1993, 1994, 1997) revealed that 23 AEs, defined as atomic environment types (AETs), are favoured. These 23 most frequently occurring AETs are shown in Fig. 9.3.4(a). In Fig. 9.3.4(b), the AETs are plotted *versus* the number of point sets investigated. Heavily preferred are the tetrahedron (CN4), the octahedron (CN6), the equatorial

tricapped trigonal prism (CN9), the icosahedron (CN12), the cubo-octahedron (CN12), and the CN14 Kasper polyhedron as AEs in intermetallic compounds. We also conclude from the observed AEs that the metallic radii that were published by Teatum *et al.* (1960) are in general not valid for intermetallic compounds. The assumption that the atoms have CN = 12 is probably never met in actual compounds. The above-mentioned



(a)

Fig. 9.3.4. (a) The 23 most frequently occurring atomic environment types (AET) with their polyhedron code (lower left corner of each box). In the upper left corner of each box, the assigned labels are given, consisting of the coordination number followed by a letter (*a*, *b*, ...). At the top right-hand corner, the crystal systems in which the AET occur are marked. (b) A frequency plot of the 23 most frequently occurring AETs *versus* the number of point sets.

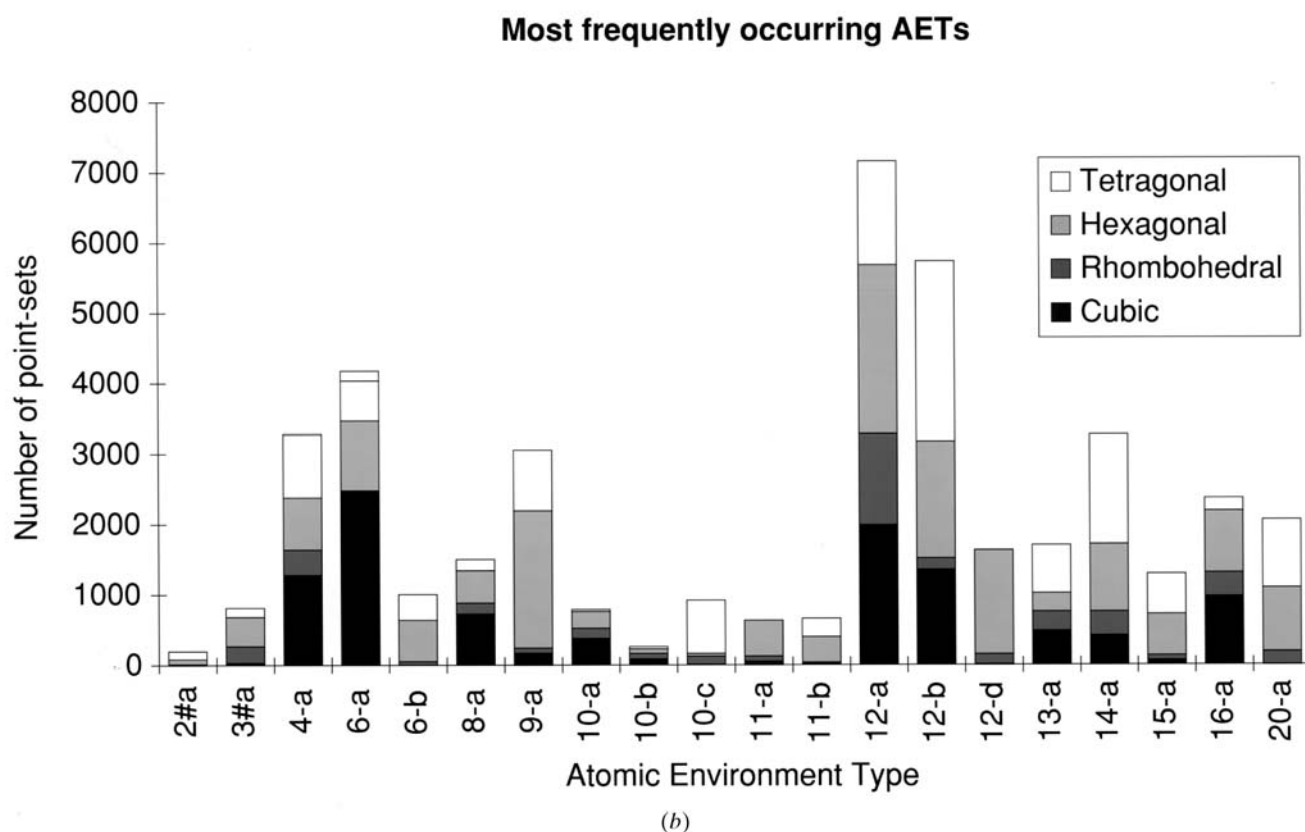


Fig. 9.3.4 (cont.)

systematic analysis shows that we have in general, especially for real intermetallic compounds, low coordination numbers,  $CN < 9$ , for the  $p$  elements,  $CN$  numbers between 9 and 14 for the  $d$  elements, and  $CN > 12$  for the  $s$  and  $f$  elements. In structure types where we have covalent or ionic bonding, we observe much lower coordination numbers. For example, the atoms of the compounds crystallizing in  $cF8$  C1Na have  $CN = 6$ , and they have the octahedron as an AE.

### 9.3.1. Glossary

**Intermetallic compound:** Intermetallic compounds are binary, ternary, quaternary, *etc.* compounds containing the chemical elements other than oxygen, the halides, and the noble gases. Also excluded are compounds containing typical inorganic groups like  $-NH$ ,  $-NH_2$ ,  $-N_2$ , *etc.* This definition was used for *Pearson's Handbook* (Villars & Calvert, 1991), the *Atlas of Crystal Structure Types* (Daams, Villars & van Vucht, 1991) and the CRYSTMET database (Rodgers & Villars, 1988). This

definition therefore also includes sulfides, selenides, carbides, and nitrides, which most material scientists would not consider to be intermetallic compounds, but, because of their structural similarity, they have been included.

**Structure type** (or prototype): Based on space-group theory, a crystal structure is completely determined by the following data: chemical formula; crystal system and unit-cell dimension(s); space group; occupation number and coordination of the occupied point sets.

Crystal structure types are named by the first intermetallic compound found to be unique in respect of the third and fourth items and are represented by the Pearson symbol followed by the formula of the prototype, *e.g.*  $hP3$  AlB<sub>2</sub>. The first two letters of the Pearson symbol are identical to the Bravais-lattice type, and the digits give the number of atoms per unit cell.