

chemical species

An ensemble of chemically identical *molecular entities* that can explore the same set of molecular energy levels on the time scale of the experiment. The term is applied equally to a set of chemically identical atomic or molecular structural units in a solid array. For example, two conformational *isomers* may be interconverted sufficiently slowly to be detectable by separate NMR spectra and hence to be considered to be separate chemical species on a time scale governed by the radiofrequency of the spectrometer used. On the other hand, in a slow chemical reaction the same mixture of conformers may behave as a single chemical species, i.e. there is virtually complete equilibrium population of the total set of molecular energy levels belonging to the two conformers. Except where the context requires otherwise, the term is taken to refer to a set of molecular entities containing isotopes in their natural abundance. The wording of the definition given in the first paragraph is intended to embrace both cases such as graphite, sodium chloride or a surface oxide, where the basic structural units may not be capable of isolated existence, as well as those cases where they are. In common chemical usage generic and specific chemical names (such as *radical* or hydroxide ion) or chemical formulae refer either to a chemical species or to a *molecular entity*.

1994, 66, 1096; 1996, 68, 2202

N.B. See also the entry for “*chemical species (of an element)*”.

IUPAC Compendium of Chemical Terminology 2nd Edition (1997)