

molecular graph

The graph with differently labelled (coloured) vertices (chromatic graph) which represent different kinds of atoms and differently labelled (coloured) edges related to different types of bonds. Within the topological electron distribution theory, a complete network of the bond paths for a given nuclear configuration.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1951