

**CPC COOPERATIVE PATENT CLASSIFICATION****G PHYSICS***(NOTES omitted)***G16 INFORMATION AND COMMUNICATION TECHNOLOGY [ICT] SPECIALLY ADAPTED FOR SPECIFIC APPLICATION FIELDS***(NOTES omitted)***G16C COMPUTATIONAL CHEMISTRY; CHEMOINFORMATICS; COMPUTATIONAL MATERIALS SCIENCE**

- 10/00** Computational theoretical chemistry, i.e. ICT specially adapted for theoretical aspects of quantum chemistry, molecular mechanics, molecular dynamics or the like
- 20/00** Chemoinformatics, i.e. ICT specially adapted for the handling of physicochemical or structural data of chemical particles, elements, compounds or mixtures
- 20/10 . Analysis or design of chemical reactions, syntheses or processes
  - 20/20 . Identification of molecular entities, parts thereof or of chemical compositions
  - 20/30 . Prediction of properties of chemical compounds, compositions or mixtures
  - 20/40 . Searching chemical structures or physicochemical data
  - 20/50 . Molecular design, e.g. of drugs
  - 20/60 . In silico combinatorial chemistry
  - 20/62 . . Design of libraries
  - 20/64 . . Screening of libraries
  - 20/70 . Machine learning, data mining or chemometrics
  - 20/80 . Data visualisation
  - 20/90 . Programming languages; Computing architectures; Database systems; Data warehousing
- 60/00** Computational materials science, i.e. ICT specially adapted for investigating the physical or chemical properties of materials or phenomena associated with their design, synthesis, processing, characterisation or utilisation
- 99/00** Subject matter not provided for in other groups of this subclass