G16C

COMPUTATIONAL CHEMISTRY; CHEMOINFORMATICS; COMPUTATIONAL MATERIALS SCIENCE

Definition statement

This place covers:

Data processing methods or systems for the storage, retrieval, analysis, distribution or visualisation of physicochemical or structural data of chemical particles, elements, compounds, or mixtures.

Computational theoretical chemistry.

Computational materials science, i.e. data processing methods or systems for investigating physics or chemistry of new or existing materials or phenomena associated with their design, synthesis, processing, characterization, or utilisation.

This subclass also covers computational chemistry and computational materials science methods or systems where the digital data processing is inherent or implicit, although not explicitly mentioned.

Relationships with other classification places

This subclass covers computational theoretical chemistry, chemoinformatics and computational materials science, whereas subclass G16B covers bioinformatics.

In order to determine whether classification should be directed to this subclass or to subclass G16B, one has to take into account the type of molecule(s), whose characterising features are processed by a computational algorithm.

Classification should be directed to subclass G16C for processing of data related to chemical entities in general, i.e. chemical particles, elements, compounds, mixtures and/or materials.

Classification should be directed to subclass G16B for processing of data related to molecules which are directly involved in molecular biology processes, i.e. molecules out of the groups of nucleic acids, proteins, peptides and amino acids.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Investigating or analysing materials by determining their chemical or physical properties	G01N
Chromatographic signal analysis	G01N 30/86
Systems controlled by a computer	G05B 15/00
Computer input/output arrangements	G06F 3/00
Computer architectures or program control	G06F 9/00
Information retrieval; Database structures therefor; File system structures therefor	G06F 16/00
Complex mathematical operations	G06F 17/10
Pattern recognition	G06F 18/00, G06V 10/00
Computer-aided design	G06F 30/00
Computer systems using neural network models	G06N 3/02

Computer systems using knowledge representation, e.g. expert systems	G06N 5/02
Computer systems using probabilistic models	G06N 7/00
Machine learning	G06N 20/00
3D image rendering	G06T 15/00
3D modelling for computer graphics	G06T 17/00
Manipulating 3D models or images for computer graphics	G06T 19/00
Bioinformatics	G16B
Healthcare Informatics	G16H
Mass spectrometry apparatus	H01J 49/00

Glossary of terms

In this place, the following terms or expressions are used with the meaning indicated:

design	Software-based creation or planning
handling	Covers retrieval, analysis, visualisation or storage
quantum chemistry	Branch of chemistry, in which quantum mechanics is applied to theoretical studies of chemical systems
molecular mechanics	Branch of chemistry, in which classical mechanics is applied to model molecular systems
molecular dynamics	Computer-based simulation method for studying movements of atoms and molecules in time by applying Newton's equations of motion and molecular mechanics force fields
in silico	Performed on a computer or via computer simulations

Synonyms and Keywords

In patent documents, the following words/expressions are often used with the meaning indicated:

systems	includes apparatus

G16C 10/00

Computational theoretical chemistry, i.e. ICT specially adapted for theoretical aspects of quantum chemistry, molecular mechanics, molecular dynamics or the like

Definition statement

This place covers:

Computer-based calculations and theoretical analysis of:

- quantum mechanics (QM), e.g. density functional theory (DFT);
- molecular mechanics (MM), e.g. details related to force fields;
- molecular dynamics (MD), e.g. details on setting up simulations;
- related Monte Carlo (MC) methods, e.g. details on MC algorithms, conformation analysis or the like.

Mere mention of modelling or simulation using QM, MM, MD, etc. is not sufficient to justify classification in this group.

G16C 20/00

Chemoinformatics, i.e. ICT specially adapted for the handling of physicochemical or structural data of chemical particles, elements, compounds or mixtures

Definition statement

This place covers:

Subject matter related to cheminformatics as specified in the subgroups.

G16C 20/10

Analysis or design of chemical reactions, syntheses or processes

Definition statement

This place covers:

Computer-assisted analysis and design of chemical reactions, processes and syntheses. The following are examples of the subjects covered:

- synthesis design;
- identifying a suitable pathway;
- reaction outcome prediction;
- crystallization/co-crystallization process prediction;
- mechanism elucidation.

G16C 20/20

Identification of molecular entities, parts thereof or of chemical compositions

Definition statement

This place covers:

Computer-assisted, measurement-based identification of molecules, parts of molecules or their molecules structures, and of compositions of multi-component mixtures, e.g. computer-assisted structure elucidation (CASE).

Computer-assisted, measurement-based, qualitative and quantitative analysis of samples.

Measurement may be based on mass spectrometry (MS), nuclear magnetic resonance (NMR), spectroscopy, chromatography, electrophoresis or the like.

G16C 20/30

Prediction of properties of chemical compounds, compositions or mixtures

Definition statement

This place covers:

Computer-assisted prediction of physical, physicochemical and biological properties of chemical compounds, compositions or mixtures. The following are examples of the subjects covered:

- computing and selecting molecular descriptors;
- computing structure-activity relationship (SAR) models;
- computing quantitative structure-activity relationship (QSAR) models;
- computing quantitative structure-property relationship (QSPR) models;

- computing absorption, distribution, metabolism, excretion and toxicity (ADME-Tox or ADMET) models; and
- computing pharmacokinetic/pharmacodynamic (PK/PD) models.

Computer-assisted prediction of a drug dosage or drug regimen.

Computer-assisted prediction of the concentration of a pharmaceutical active agent/drug based on molecular data, wherein the drug/active agent can be any molecule other than in the group of nucleic acids, proteins, peptides and their conjugates.

G16C 20/40

Searching chemical structures or physicochemical data

Definition statement

This place covers:

Database search of chemical structures or physicochemical data. The following are examples of the subjects covered:

- full structure search;
- substructure search;
- similarity search;
- combinations of similarity coefficients;
- pharmacophore search; and
- 3D structure search.

G16C 20/50

Molecular design, e.g. of drugs

Definition statement

This place covers:

Computer-assisted design and modelling of molecules to be used for any purpose. The following are examples of the subjects covered:

- drug design with the emphasis on a therapeutic agent;
- ligand-biological target interactions;
- docking algorithms, and pharmacophore generation.

Computer-assisted drug formulation.

G16C 20/60

In silico combinatorial chemistry

Definition statement

This place covers:

In silico designing and screening of combinatorial chemical libraries of compounds other than nucleic acids, proteins, peptides, or amino acids.

Mere mention of combinatorial libraries of particular types of compounds is not sufficient to classify in this place.

G16C 20/70

Machine learning, data mining or chemometrics

Definition statement

This place covers:

Computer-assisted discovery and/or analysis of patterns within a vast amount of physicochemical data, wherein the emphasis is placed on the methods of analysis and is largely independent of the particular type of physicochemical data.

Analysis methods are based on any of:

- machine learning;
- statistical models;
- supervised and unsupervised learning techniques;
- pattern finding;
- knowledge discovery;
- rule extraction;
- correlation;
- clustering; and
- classification.

G16C 20/80

Data visualisation

Definition statement

This place covers:

Visual representations specifically adapted to structural and/or physicochemical data, wherein the emphasis is placed on the method of visualisation and is largely independent of the particular type of structural and/or physicochemical data.

The following are examples of the subjects covered:

- graphics generation;
- map display (e.g. physical and/or chemical properties maps);
- chemical structure representations (e.g. chemical name-to-structure conversion algorithms).

G16C 20/90

Programming languages; Computing architectures; Database systems; Data warehousing

Definition statement

This place covers:

Software specially adapted to assist in programming procedures within computational chemistry.

Encryption and compression algorithms specially adapted for chemical data, e.g. chemical fingerprints.

Database systems specially adapted for managing chemical data.

The following are examples of the subjects covered:

- ontologies;
- heterogeneous data integration;

- data warehousing;
- computing architectures.

G16C 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

Definition statement

This place covers:

Computer-assisted mathematical modelling of the structures (e.g. metals, polymers, ceramics, composites, biomaterials, nanomaterials) by applying the knowledge of physics, physical chemistry and chemistry.

In particular modelling of:

- structures of materials (e.g. structural defects and their resulting limitations);
- properties of materials (e.g. electronic, thermal, chemical, magnetic, optical); and/or
- behaviors of materials.

Computer-assisted investigation of existing materials and design of new ones.

Computational investigation of existing materials and design of new ones.