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

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

20/50 . Molecular design, e.g. of drugs20/60 . <u>In silico</u> 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

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