

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	20/70	. Machine learning, data mining or chemometrics
		20/80	. Data visualisation
		20/90	. Programming languages; Computing architectures; Database systems; Data warehousing
	WARNING	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
	Group G16C 10/00 is incomplete pending reclassification of documents from group G16C 99/00 .		WARNING
	Groups G16C 99/00 and G16C 10/00 should be considered in order to perform a complete search.		Group G16C 60/00 is incomplete pending reclassification of documents from group G16C 99/00 .
20/00	Chemoinformatics, i.e. ICT specially adapted for the handling of physicochemical or structural data of chemical particles, elements, compounds or mixtures		Groups G16C 99/00 and G16C 60/00 should be considered in order to perform a complete search.
	WARNING	99/00	Subject matter not provided for in other groups of this subclass
	Groups G16C 20/00 – G16C 20/50 , G16C 20/70 – G16C 20/90 are incomplete pending reclassification of documents from group G16C 99/00 .		WARNING
	All groups listed in this Warning should be considered in order to perform a complete search.		Group G16C 99/00 is impacted by reclassification into groups G16C 10/00 , G16C 20/00 , G16C 20/10 , G16C 20/20 , G16C 20/30 , G16C 20/40 , G16C 20/50 , G16C 20/60 , G16C 20/62 , G16C 20/64 , G16C 20/70 , G16C 20/80 , G16C 20/90 , and G16C 60/00 .
20/10	. Analysis or design of chemical reactions, syntheses or processes		All groups listed in this Warning should be considered in order to perform a complete search.
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	. <i>In silico</i> combinatorial chemistry		
	WARNING		
	Group G16C 20/60 is incomplete pending reclassification of documents from group G16C 99/00 .		
	Group G16C 20/60 is also impacted by reclassification into groups G16C 20/62 and G16C 20/64 .		
	All groups listed in this Warning should be considered in order to perform a complete search.		
20/62	. . Design of libraries		
20/64	. . Screening of libraries		