

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 20/80 20/90	<ul style="list-style-type: none"> Machine learning, data mining or chemometrics Data visualisation Programming languages; Computing architectures; Database systems; Data warehousing
	WARNING Group G16C 10/00 is incomplete pending reclassification of documents from group G16C 99/00 . Groups G16C 99/00 and G16C 10/00 should be considered in order to perform a complete search.	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 WARNING Group G16C 60/00 is incomplete pending reclassification of documents from group G16C 99/00 . Groups G16C 99/00 and G16C 60/00 should be considered in order to perform a complete search.
20/00	Chemoinformatics, i.e. ICT specially adapted for the handling of physicochemical or structural data of chemical particles, elements, compounds or mixtures WARNING Groups G16C 20/00 – G16C 20/50 , G16C 20/70 – G16C 20/90 are incomplete pending reclassification of documents from group G16C 99/00 . All groups listed in this Warning should be considered in order to perform a complete search.	99/00	Subject matter not provided for in other groups of this subclass WARNING 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 . All groups listed in this Warning should be considered in order to perform a complete search.
20/10	<ul style="list-style-type: none"> Analysis or design of chemical reactions, syntheses or processes 		
20/20	<ul style="list-style-type: none"> Identification of molecular entities, parts thereof or of chemical compositions 		
20/30	<ul style="list-style-type: none"> Prediction of properties of chemical compounds, compositions or mixtures 		
20/40	<ul style="list-style-type: none"> Searching chemical structures or physicochemical data 		
20/50	<ul style="list-style-type: none"> Molecular design, e.g. of drugs 		
20/60	<ul style="list-style-type: none"> <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	<ul style="list-style-type: none"> Design of libraries 		
20/64	<ul style="list-style-type: none"> Screening of libraries 		