

# 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	<b>Computational theoretical chemistry, i.e. ICT specially adapted for theoretical aspects of quantum chemistry, molecular mechanics, molecular dynamics or the like</b>	20/70	• Machine learning, data mining or chemometrics
		20/80	• Data visualisation
		20/90	• Programming languages; Computing architectures; Database systems; Data warehousing
	<b><u>WARNING</u></b>	60/00	<b>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</b>
	Group <a href="#">G16C 10/00</a> is incomplete pending reclassification of documents from group <a href="#">G16C 99/00</a> .		<b><u>WARNING</u></b>
	Groups <a href="#">G16C 99/00</a> and <a href="#">G16C 10/00</a> should be considered in order to perform a complete search.		Group <a href="#">G16C 60/00</a> is incomplete pending reclassification of documents from group <a href="#">G16C 99/00</a> .
20/00	<b>Cheminformatics, i.e. ICT specially adapted for the handling of physicochemical or structural data of chemical particles, elements, compounds or mixtures</b>		Groups <a href="#">G16C 99/00</a> and <a href="#">G16C 60/00</a> should be considered in order to perform a complete search.
	<b><u>WARNING</u></b>	99/00	<b>Subject matter not provided for in other groups of this subclass</b>
	Groups <a href="#">G16C 20/00</a> – <a href="#">G16C 20/50</a> , <a href="#">G16C 20/70</a> – <a href="#">G16C 20/90</a> are incomplete pending reclassification of documents from group <a href="#">G16C 99/00</a> .		<b><u>WARNING</u></b>
	All groups listed in this Warning should be considered in order to perform a complete search.		Group <a href="#">G16C 99/00</a> is impacted by reclassification into groups <a href="#">G16C 10/00</a> , <a href="#">G16C 20/00</a> , <a href="#">G16C 20/10</a> , <a href="#">G16C 20/20</a> , <a href="#">G16C 20/30</a> , <a href="#">G16C 20/40</a> , <a href="#">G16C 20/50</a> , <a href="#">G16C 20/60</a> , <a href="#">G16C 20/62</a> , <a href="#">G16C 20/64</a> , <a href="#">G16C 20/70</a> , <a href="#">G16C 20/80</a> , <a href="#">G16C 20/90</a> , and <a href="#">G16C 60/00</a> .
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		
	<b><u>WARNING</u></b>		
	Group <a href="#">G16C 20/60</a> is incomplete pending reclassification of documents from group <a href="#">G16C 99/00</a> .		
	Group <a href="#">G16C 20/60</a> is also impacted by reclassification into groups <a href="#">G16C 20/62</a> and <a href="#">G16C 20/64</a> .		
	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		