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- as to applicant's entitlement to apply for and be granted a patent (Rule 4.17(ii))
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(54) Title: CHEMICAL REACTION GRAPH ENCODING SOFTWARE, CORRESPONDING METHOD AND ASSOCIATED DATA APPLICATIONS

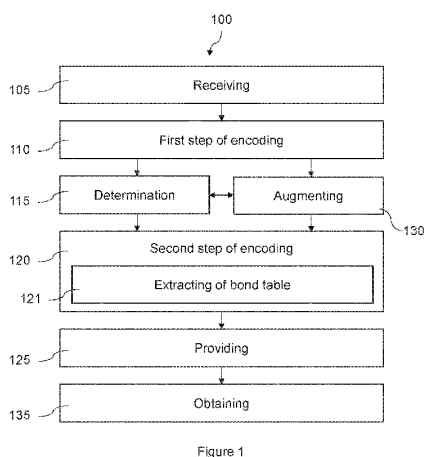


Figure 1

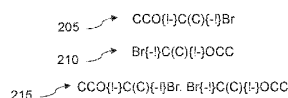


Figure 2

(57) Abstract: The chemical reaction encoding method (100) for one-step, multi-step and equilibrium reactions, comprises: - a step (105) of receiving, upon a computer interface, a chemical reaction graph comprising at least one chemical reaction reagent and at least one chemical reaction product, - a first step (110) of encoding, by a computing device, said chemical reaction graph describing the structure of at least one said reagent and said product, - a step (115) of determination, by a computing device, of changing bonds within the encoding representative of the chemical structures of at least one said reagent and said product, - a second step (120) of encoding, by a computing device, in a single string of characters, for at least one changing bond determined, at least one character representative of an atom subject to the change of bond, at least one character representative of the type of changing bond determined and at least one character representative of an atom resulting from the change of bond, in which a changing bond is encoded by a set of two characters representative of the changing bond determined, the first character being representative of the reagent bond and the second character being representative of the product bond, each character being selected in a library of bijective characters wherein one character is representative of one changing bond type and - a step (125) of providing, upon a computer interface, the string of characters corresponding to the encoding of changing bonds of the chemical reaction.

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