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Consensus approach to atom-to-atom mapping in chemical reactions

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Abstract

In this paper, new methodology of atom-to-atom mapping (AAM) in chemical reactions based on consensus of different algorithms was proposed. Principle of minimal chemical distance is the cornerstone of the methodology. Original formulation of the principle was made applicable to stoichiometrically unbalanced reactions using conception of Condensed Graph of Reaction. In the framework of proposed methodology two approaches for AAM refinement was proposed: sequential approach that could be used for reaction of known type, and parallel approach, applicable to reaction datasets of unknown mechanism. It was shown that both approaches reduce the number of errors in AAM. Parallel approach was used to find AAM in ChemSpider Reactions dataset and quality of the mapping was verified.