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Presentation of chemical reactions, reagents and their thermo-chemical properties in the intelligence system on physical chemistry of liquid phase radical reactions with the use of the ontological model of the domain

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Abstract

In this paper a fragment of the domain ontology on physical chemistry of liquid phase radical reactions is presented. The presented ontological model of the domain includes about 100 subclasses of radical reactions, more than 50 classes of organic compounds and about 45000 object properties (physical and chemical properties of molecules, radicals and radical reactions). The ontology is developed with the use of ontology editing tool Protégé. The ontology will be used in the scientific intelligence system on physical chemistry of radical reactions.