

InChI meta data with kfile_chemical

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Kde, Inchi

Abstract

I've just uploaded kfile_chemical 0.9 . It has new translations for ES and DA, and plugins for InChI files. It will extract the InChI string as meta data (and will thus be used by the KDE desktop search Kat , and the InChI version number.

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chem-bla-ics

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Thinking about this, it might be useful to extract all layers as meta data, so that one can search on chemical formula and even connectivity, and find all matching structures. Not really close to substructure search, but we'll tackle that later :)