chem-bla-ics

More chemistry in KDE

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Published March 11, 2006

Citation
Willighagen, E. (n.d.). In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/83mgj-93w85

Keywords
Kde, Chemistry

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After Kalzium and kfile_chemical , KDE has now be extended with kparts for 3D structure and spectrum display: Kryomol . It is written in C++ and licensed GPL. It supports several chemistry formats, among which quantum chemical formats like Gaussian03, NwChem and ACES, and 3D structures as MDL molefile and XYZ.