More chemistry in KDE

Egon Willighagen ⬤

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Abstract

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.

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