

24. Migration

Going from one CDK release to another brings in API changes. While the project tries to keep the number of changes minimal, these are inevitable. This chapter discusses some API changes, and shows code examples on how to change your code. Section 24.1 discusses changes from 1.2 to 1.4, Section 24.2 discusses changes from 1.0 to 1.2, and Section 24.3 discusses changes from 1.0 to 1.4.

The set of changes include changed class names. For example, the CDK 1.2 class `MDLWriter` is now called `MDLV2000Writer` to reflect the V2000 version of the MDL formats.

24.1. CDK 1.4 to 1.6

This section highlights the important API changes between the CDK 1.4 and 1.6 series.

24.1.1. Removal of the `NoNotify` interface implementation

The `NoNotificationChemObjectBuilder` and the matching implementation classes are removed. Please use the `SilentChemObjectBuilder` instead.

24.1.2. Removal of `IMolecule`

The `IMolecule` interface and all implementing classes have been removed. They were practically identical in functionality to the `IAtomContainer` interface, except the implication that the `IMolecule` was for fully connected structures only. This separation was found to be complicated, and was therefore removed. Please use the `IAtomContainer` interface instead.