
atomium Documentation

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atomium is a molecular modeller and file parser.

CHAPTER 1

Example

```
>>> import atomium
>>> glucose = atomium.xyz_from_file("glucose.xyz")
>>> glucose.comment()
'glucose from 2gbbp'
>>> glucose.model()
<Model (12 atoms)>
>>> glucose.model().mass()
168.0606
```


CHAPTER 2

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