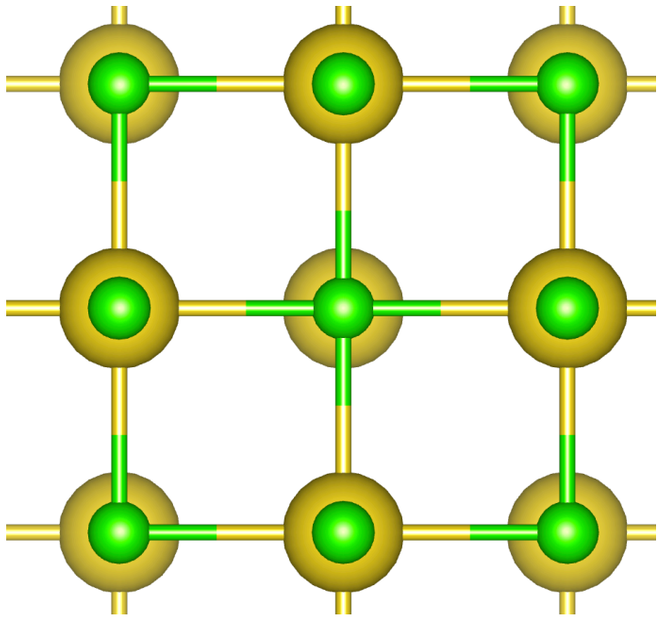
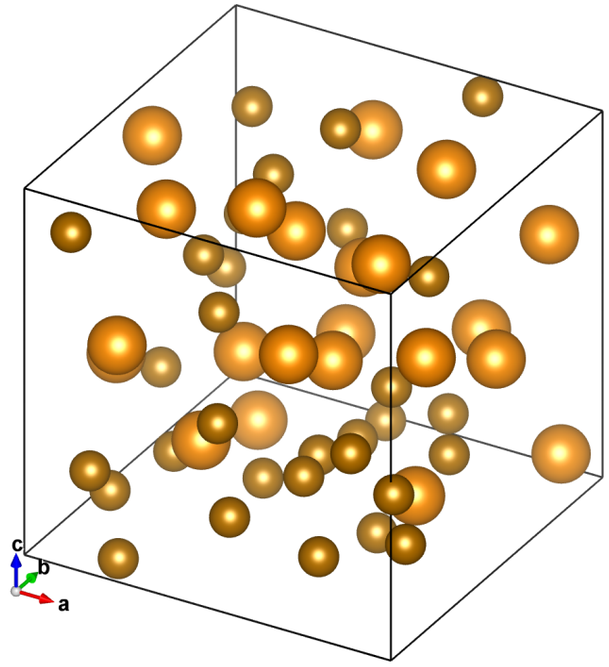
Atomic coordinates to atomic bonding graphs: exploration of data-scientific treatment

Materials Design Group
2nd Innovation Camp of
Computational Materials Science
Oct. 4th, 2018

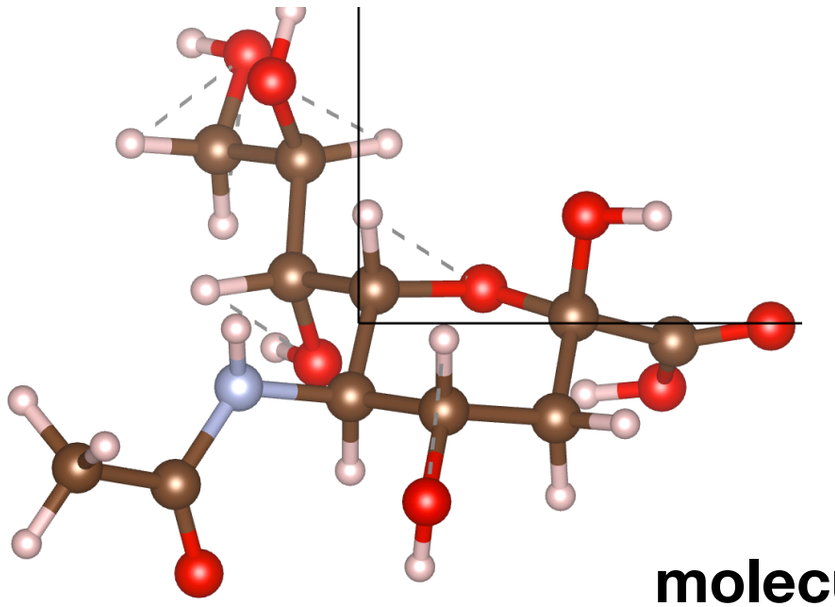
Extraction of information from atomic coordinates



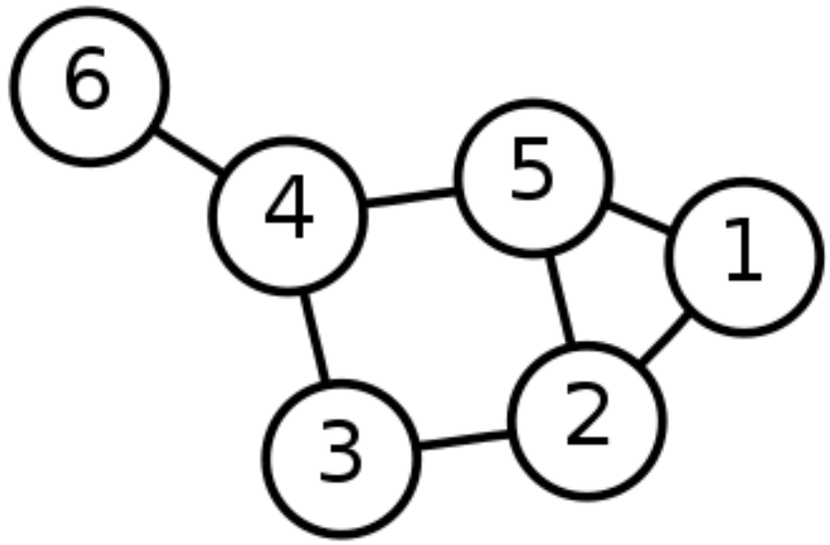
crystal?



amorphous?

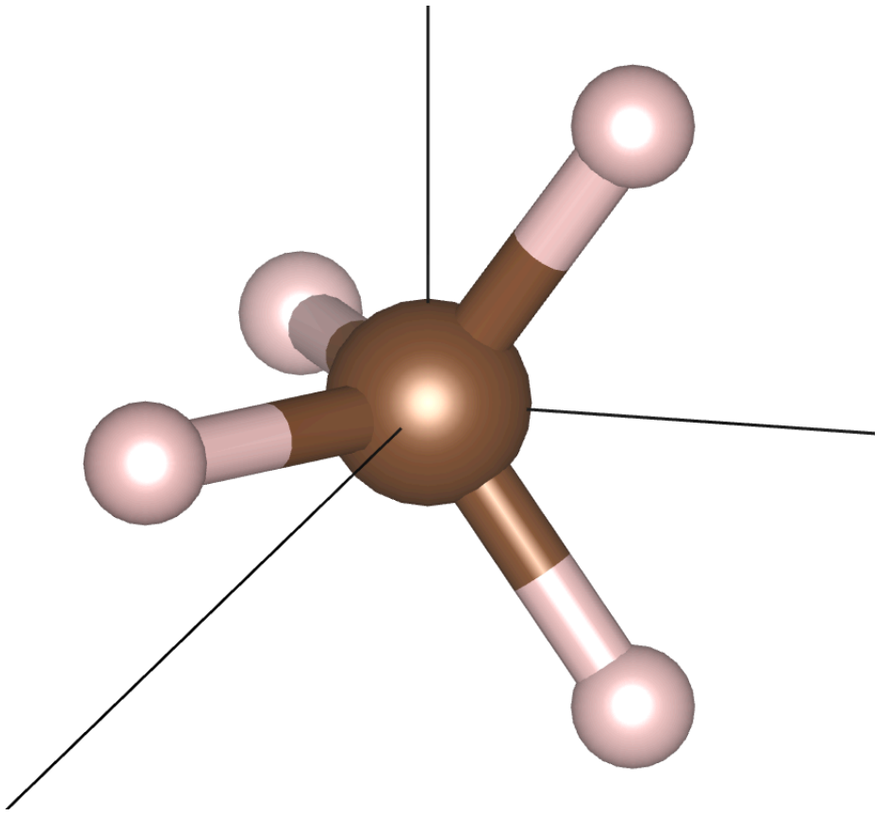


molecule?



Conversion to graphs!

Atomic bonding graph



Atomic coordinates (sample input of OpenMX)

```
1    C      2    H      1.09
1    C      3    H      1.09
1    C      4    H      1.09
1    C      5    H      1.09
                .....
```

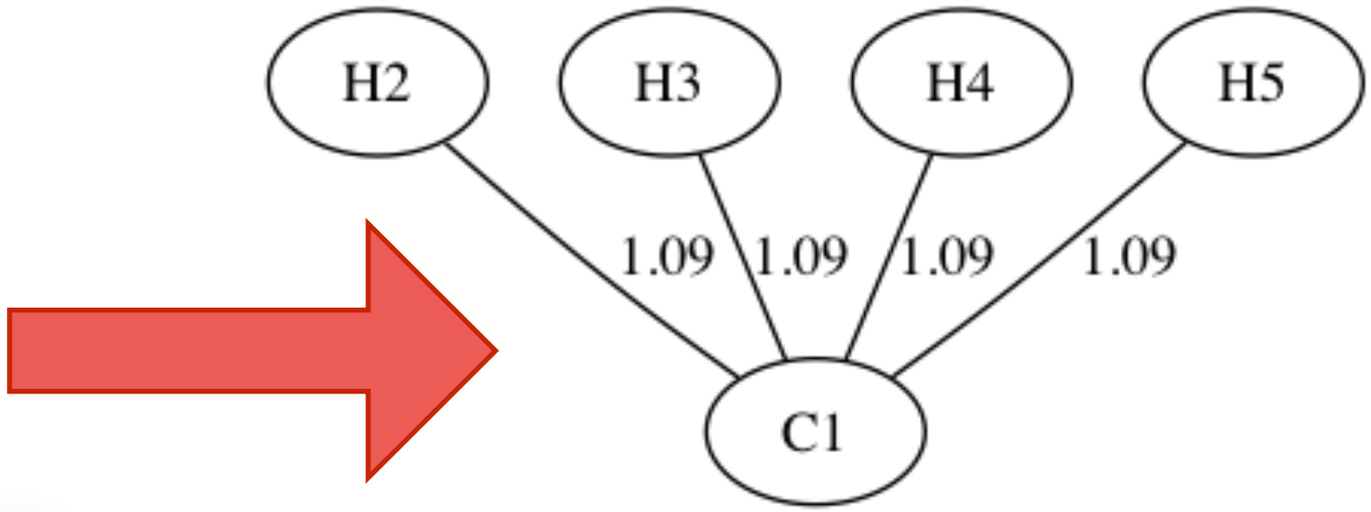
Corresponding graphs treatable by libraries

- Determine atomic bonding by comparing with cut-off distances

$$d_{\mathrm{AB}} < r_{\max}(\mathrm{A}) + r_{\max}(\mathrm{B})$$

Boost Graph Library (1)

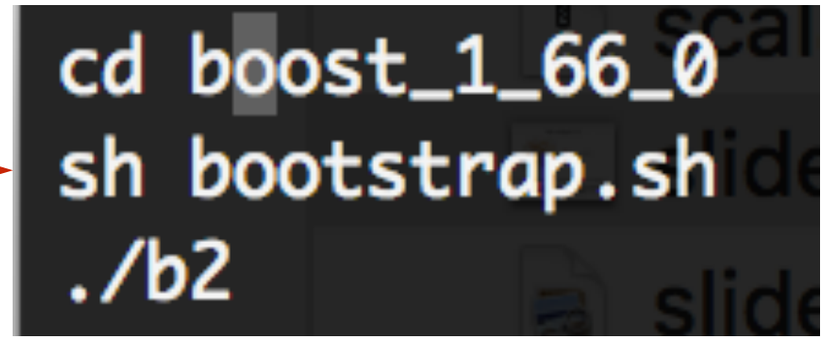
```
1    C        2    H      1.09
1    C        3    H      1.09
1    C        4    H      1.09
1    C        5    H      1.09
                .....
```



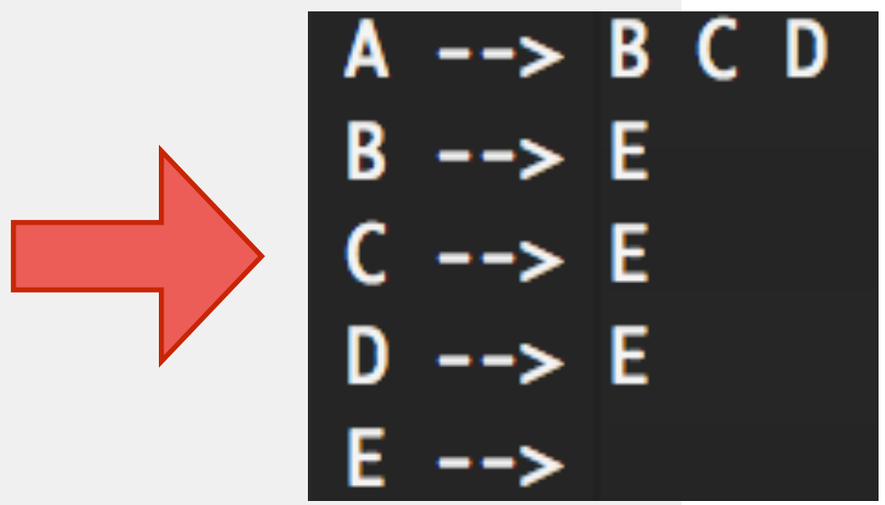
- Generate graphs from atomic coordinates and/or any physical systems
- Analyze those graphs using Boost Graph Library
- **https://www.boost.org/**
- Detailed Japanese instructions in **https://boostjp.github.io/**

Boost graph Library (2)

- Installation
- Test program (from boostjp)

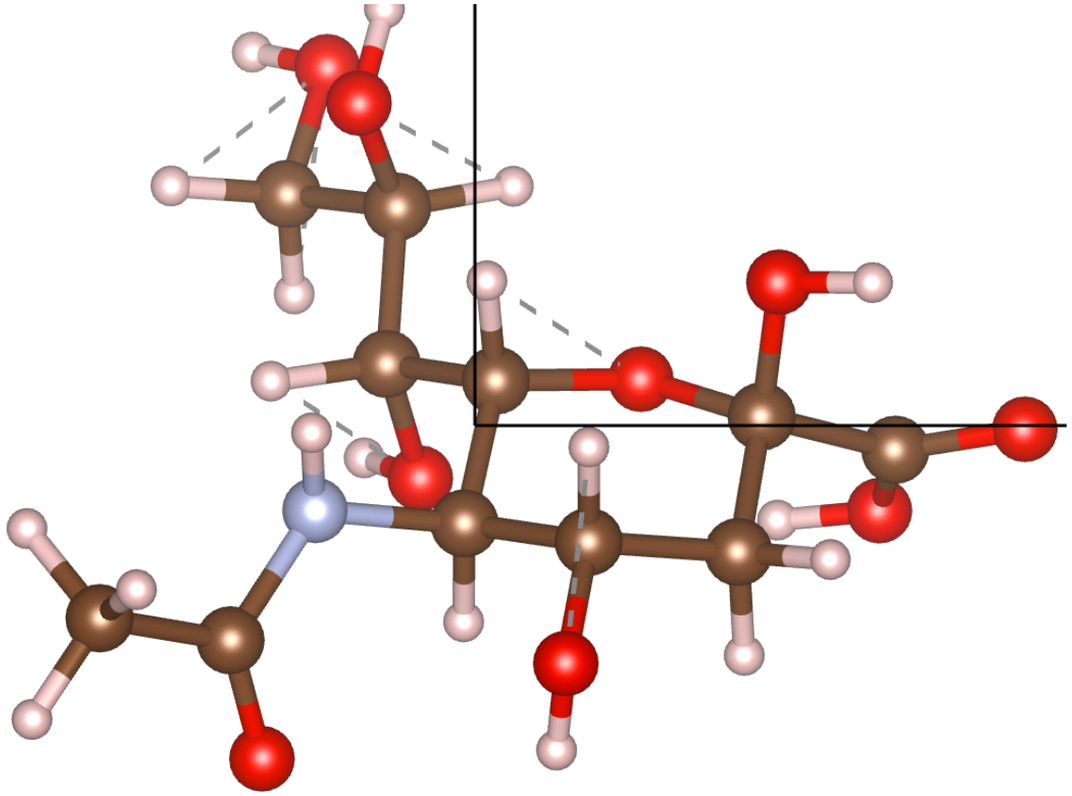



```cpp
#include <utility>
#include <string>
#include <boost/graph/adjacency_list.hpp>
#include <boost/graph/graph_utility.hpp>

typedef boost::adjacency_list<boost::listS, boost::vecS, boost::directedS> Graph;
typedef std::pair<int, int> Edge;

enum { A, B, C, D, E, N };
const std::string name = "ABCDE";

int main()
{
    const std::vector<Edge> edges = {
        {A, B}, {A, C}, {A, D},
        {B, E}, {C, E}, {D, E}
    };

    const Graph g(edges.begin(), edges.end(), N);

    boost::print_graph(g, name.c_str());
}
```

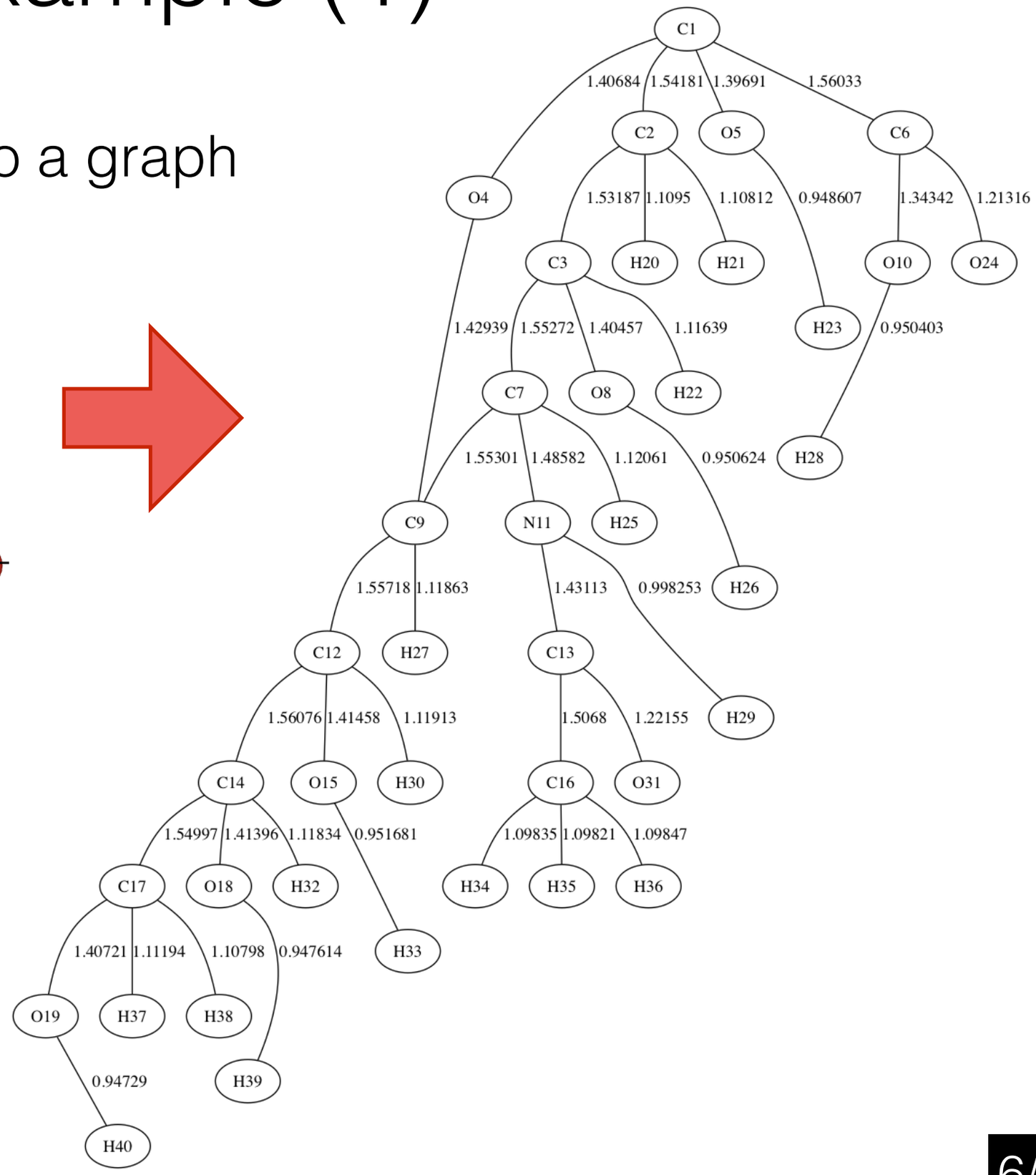


Example (1)

- Convert a molecule into a graph

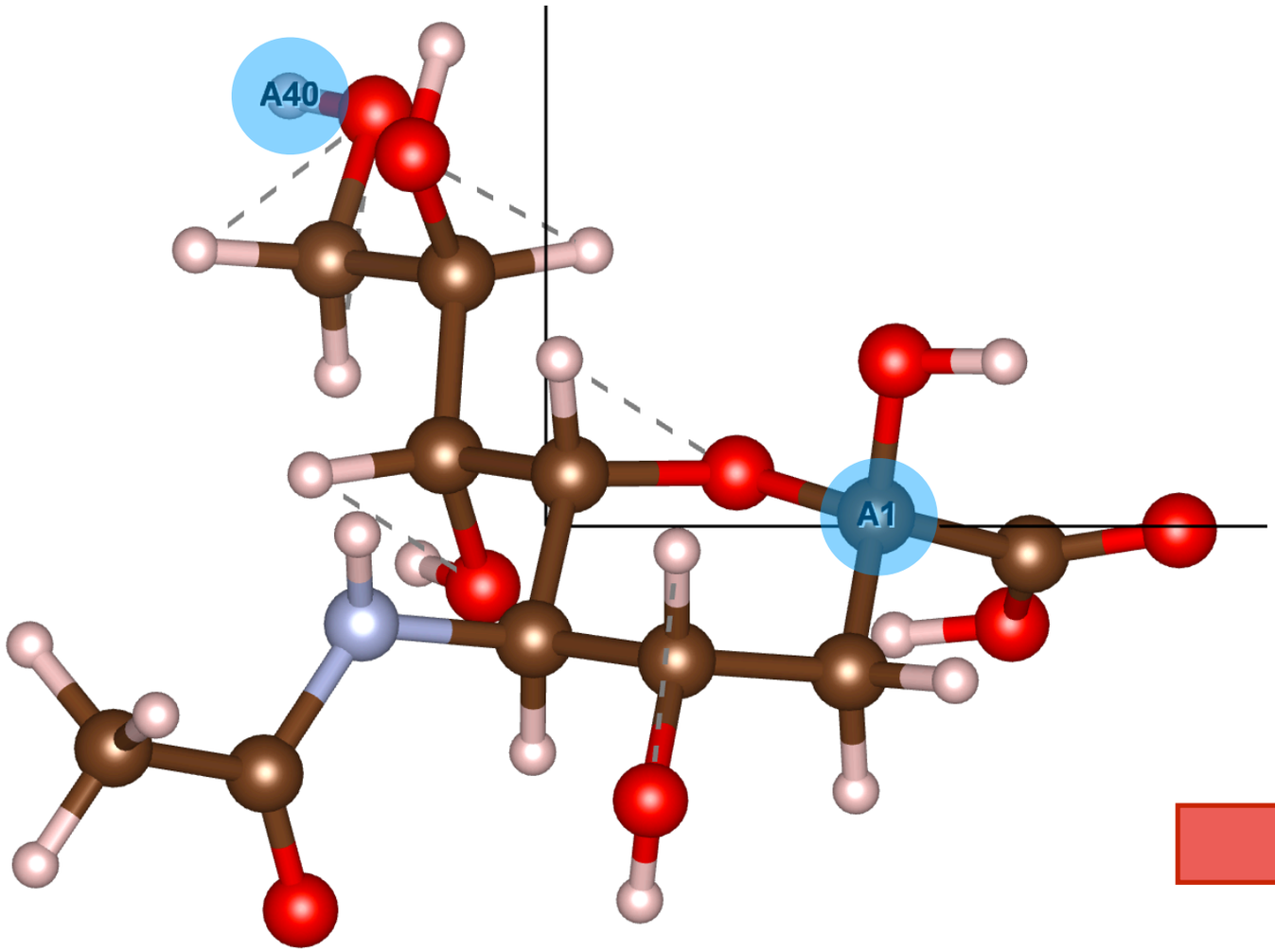


Sialic acid
(from sample input of OpenMX)

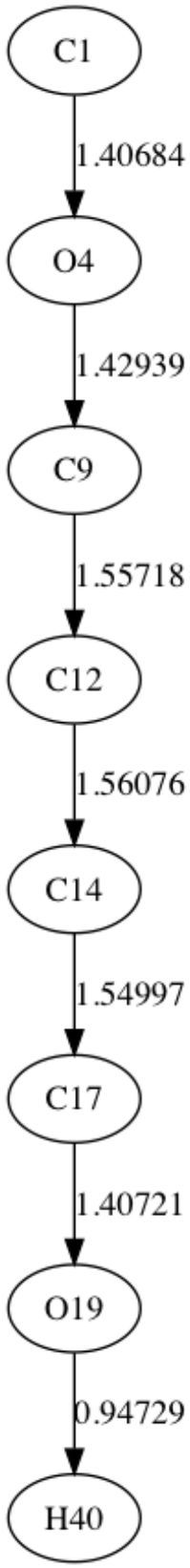


Example (2)

- Extraction of shortest path



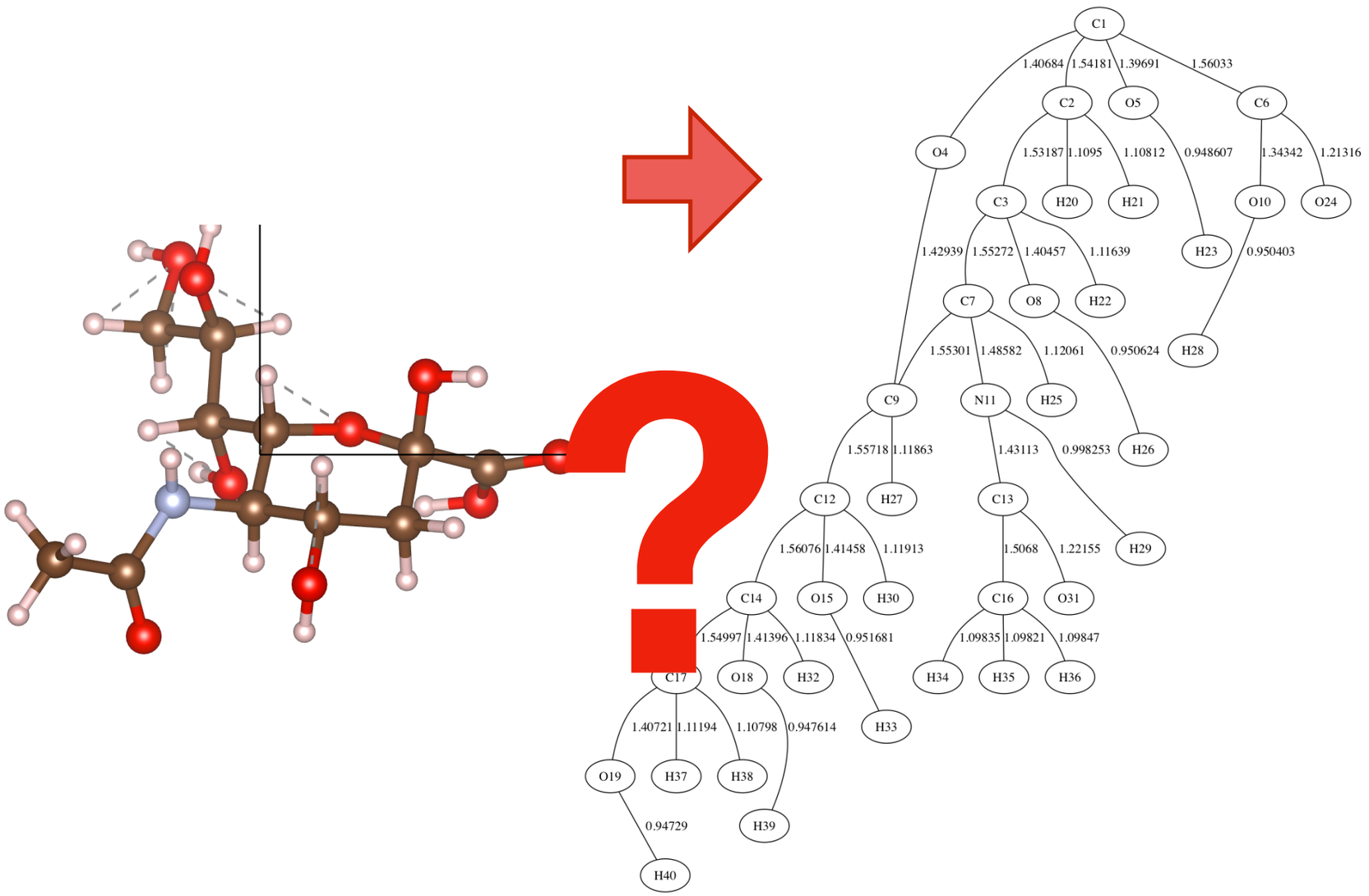
a



route length: 9.85865

Our proposal…

- Prepare graph data by text file from atomic coordinates!
- Then read it by c++ program!
- Use Boost library, then we can do something… (?)



Possible application to materials design

- Analysis of **molecular conduction**?
  - Effective electron paths should be important!