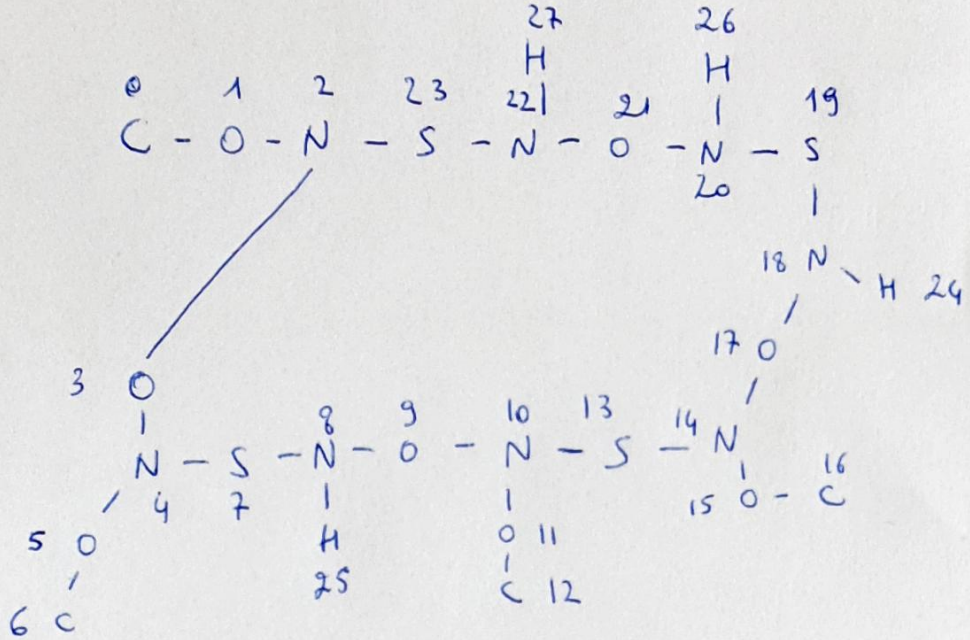
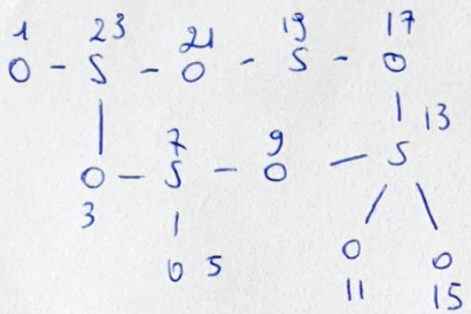
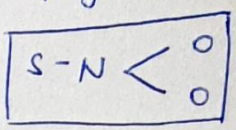




Crucial topological element:



Purpose: reduce the granularity of the bond adjacency list by eliminating all C, N and H atoms. Whenever an N atom is deleted, its "O" neighbors (if any) should be linked to the nearest S.

Strategy: begin DFS from S;
if either H or O is encountered, return;
if O, add O to S's neighbor list and S to O's.
Iterate over all S atoms.

↓ Scale up this reasoning to the DGEBA/DDS rgs

There's only 1 problem: while there is a 1-to-1 map between DDS and S atoms, there isn't one between DGEBA and O atoms.

⇒ Associate each DGEBA molecule with its central C atom, which is the only one bonded to 4 C atoms.

Purpose: Compact DGEBA into a single vertex and DDS into a single vertex, while preserving the connectivity of the network.

↑
Cross-link