

# Algorithm: Molecular Graph Realizability Check

**Input:** A sequence of integer sets  $C = \{E_1, E_2, \dots, E_n\}$ , where each set  $E_i = \{v_{i1}, v_{i2}, \dots, v_{im_i}\}$  is sorted in ascending order.

**Output:** Boolean value indicating whether  $C$  is realizable as a molecular graph.

## Procedure:

### Initialization:

Set  $C_{max} = \{d_1, d_2, \dots, d_n\}$ , such that  $d_i \leftarrow \max(E_i)$ , for all  $i$

Compute total valence sum:  $D = \sum_{i=1}^n d_i$

### Step 1: Handshake Lemma Check

if  $D$  is odd then

Iterate over  $C$  to find odd  $\Delta$  such that  $\Delta = d_i - v_{ij}$  for  $v_{ij} \in E_i \setminus \{d_i\}$ . If multiple odd  $\Delta$  exist, take the smallest one.

if such odd  $\Delta$  exists for any first  $E_i$  then

Update max valence:  $d_i \leftarrow d_i - \Delta$ , update sum:  $D \leftarrow D - \Delta$

else

Return false

end if

end if

### Step 2: Connectivity Check

if  $D < 2(n - 1)$  then

Return false

end if

### Step 3: Loop Prevention Check

if  $D \geq 2d_{imax}$ , where  $d_{imax} = \max\{d_1, d_2, \dots, d_n\}$  then

Return true

else

if  $v_{ij} < d_{imax}$  exists in  $E_i$  then

Update  $C$ : remove  $d_{imax}$  from  $E_i$

Set  $v_{imax} \leftarrow$  next largest available  $v_{ij}$

Update  $C_{max}$ : replace  $d_{imax}$  with  $v_{imax}$

Update sum:  $D \leftarrow D - d_{imax} + v_{imax}$

Go to Step 1

else

Return false

end if

end if