

Algorithm: Molecular Graph Realizability Check

Input: A sequence of integer sets $S = \{V_1, V_2, \dots, V_n\}$, where each $V_i = \{v_{i1}, v_{i2}, \dots, v_{im}\}$ is a set of possible valences for chemical element i , sorted in ascending order.

Output: Boolean value indicating whether the sequence is realizable as a molecular graph.

Procedure:

Initialization:

Select the maximum valence for each element: $d_i \leftarrow \max(V_i)$ for all i

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

Step 1: Handshake Lemma Check

if D is odd **then**

Find the smallest Δ such that $\Delta = d_i - v_j$ for some $v_j \in V_i \setminus \{d_i\}$, sequentially checking the largest possible v_j until Δ is odd.

if such a Δ exists for any i **then**

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

else

Reject sequence

end if

end if

Step 2: Connectivity Check

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

Reject sequence

end if

Step 3: Loop Prevention Check

if $D \geq 2 \max\{d_1, d_2, \dots, d_n\}$ **then**

Accept sequence as realizable

else

Identify the set of indices $I = \{j \mid d_j = \max(d_i)\}$

Select an index $i \in I$ where $d_i \neq d_{i+1}$, if such exists

if a lower valence exists in V_i **then**

Reduce d_i to the next largest available valence in V_i

Update D and recurse with the modified sequence

else

Reject sequence

end if

end if