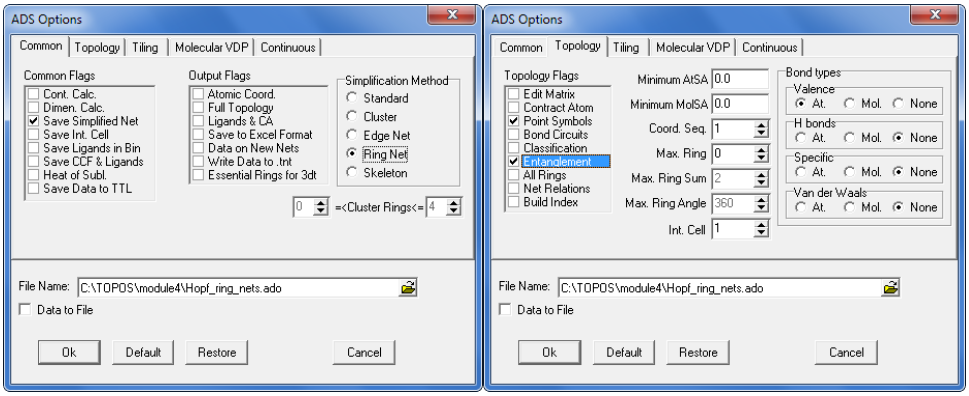
Example 5: building Hopf ring net for the crystal structure of GULBAR, [Zn(atz)(isonic)]·0.5Hisonic, atz = 5-amino-tetrazolate, Hisonic=isonicotinic acid.

Algorithm:

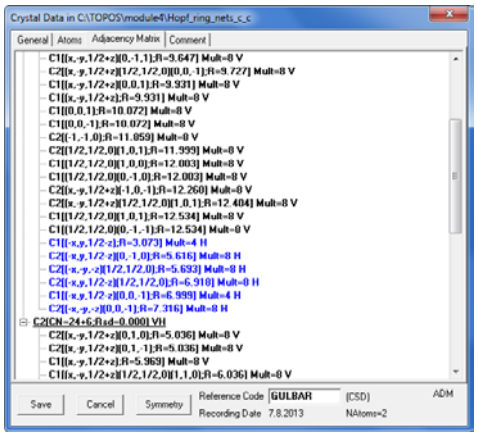
(1) Open the database **Hopf_ring_nets** and compute the adjacency matrices for the crystal structure (default parameters for AutoCN).

(2) Build standard representation for the record GULBAR. Be sure that the resulting simplified net consists of 4-coordinated Zn atoms. (do not forget to remove 2-c nodes by means of the Simplify Adjacency Matrix procedure)

(3) For the simplified structure run ADS in the **Ring Net** simplification mode with the following options specified (remember to select all atoms as "central atoms"):



(4) Open **Crystal Data** window for the simplified structure and be sure that there are six links marked as "H bonds" per each ring center (node of the ring net).



Using the ADS classification mode (see Module 5) you may determine the topology of the Hopf ring net (the net of H bonds) as 6-c **hxg**. (Tip: set in **Topology/Bond Types**: H-bonds: **At. /** Valence: **None**)

Exercise: simplify another structure in the **Hopf_ring_nets** database (LAYKOM). Build a Hopf ring net for LAYKOM. Does the coordination of nodes in the Hopf ring net differ from GULBAR? Is the topology of 2-fold interpenetration of the diamondoid nets the same in GULBAR and LAYKOM?

Answer: HRN for LAYKOM consist of 6-c and 10-c nodes (in ratio 1:1), while HRN for GULBAR is constructed with only 6-c nodes, so their topologies (rather as topology of interpenetration) are completely different. This shows different modes of entanglements for **dia** nets rings.

For more details on Hopf Ring Nets see "A topological method for classification of entanglements in crystal networks" E. V. Alexandrov, V. A. Blatov and D. M. Proserpio, *Acta Cryst.*, **A68**, 2012, 484-493.