How to create an *nnt* file for the *topcryst* services with *ToposPro*?

1. Check if you have downloaded the *TTD* Collection. For this purpose go to the **Database/TTD Collection** part of the *ToposPro* menu and click the **Clear** item to remove the *TTD* Collection from memory. If the **Clear** item is not active, no action is required.

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2. Select (using **Ins** or **Shift-Down/Up** keys) the record in the database with the net, for which the topology should be determined.

3. Open an *ADS* window and go to the **Options**.

4. Click the **Default** button in order to clear all the options used for previous calculations. In the **Common** tab, check the **Data on New Nets** flag.

ADS Options		×	
Common Topology Tiling Common Flags □ Cont. Calc. Image: Cont. Calc. □ Save Simplified Net Image: Save Simplified Net □ Save Simplified Net Image: Save Int. Cell □ Save Ligands in Bin Image: Save CCF & Ligands □ Heat of Subl. Image: Save Data to TTL □	Molecular VDP Continuous Output Flags Atomic Coord. Full Topology Ligands & CA Save to Excel Format V Data on New Nets Write Data to .tnt Essential Rings for 3dt	Simplification Method Standard Cluster Edge Net Ring Net Skeleton	
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5. Answer **Yes** to the question in the appeared window.

Confirm	×
?	You have to check 'Dimen. Calc.', 'Classification' flags, and set 'Max. Ring' to non-zero value. Make this changes now?
	Yes No

- 6. Check also Cont. Calc. option.
- 7. Press **Ok** button in the ADS options and run the calculation.
- 8. Answer **No** to the request for loading the *TTD* Collection.



9. The *nnt* file will appear in the database directory. This file contains topological indices that characterize the topology of the net with a high precision. An example of the contents of the *nnt* file is as follows:

```
'$6T1',
'{4^12.6^3}',
'6 18 38 66 102 146 198 258 326 402',
'[4.4.4.4.4.4.4.4.4.4.4.6(4).6(4).6(4)]',
'[4.4.4.4.4.4.4.4.4.4.4.*.*.*]',
```

10. Upload this file to the *topcryst* service to determine the topology of the net.