## Thymidin Invariom Transfer and Multipole Refinemet of a 20K Data Set, a Comparison

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Nucleosides play a key role in life. Therefore they are interesting compounds for X-Ray charge density studies, because this would help to understand their biological function in more detail. The invariom aproach[1] uses small theoretically calculated model compounds to derrive the multipole populations without the need of high resolution data, because they are kept unrefined.

Thymidin, which is one of the DNA nucleosides, was measured at 20K with Mo-K<sub>a</sub> radiation up to a resolution of  $\sin\theta/\lambda=1.1$ Å<sup>-1</sup>. After the spherical refinement of the structure a multipole refinement was executed and also the recently developed invariom transfer was applied. A topological analysis was done in both approaches.

The results of the invariom transfer, the multipole refinement and the theoretical calculations were compared to have a better guess about the quality of the new approach.

[1] Dittrich B., Korisánszky T., Luger P., Angew. Chem. Int. Ed., 2004, 38, 1397.

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