MS28-P11 Anharmonic thermal motion in glutathion investigated by the Maximum-Entropy-Method (MEM)

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γ-*L*-Glutamyl-*L*-cysteinyl-glycine (Glutathion) was measured at 100K using MoK$_\alpha$ radiation. A dynamic electron density map was calculated by the PRIOR[1] program of the BayMEM[2] suite and used for the Maximum-Entropy-Method calculation. As a model for this prior density Invarioms[3] with harmonic ADP's were applied. In the Invariom refinement for the prior model coordinates and harmonic ADP's were refined and multipole parameters were taken from the data-base.

A previous Invariom refinement refining Gram-Charlier parameters up to 3rd order on the carboxyl oxygen atoms of the glycine part of the molecule led to probability density function with significant negative values. The MEM can not produce such artefacts. We show the effect of the anharmonic motion on the dynamic electron density.

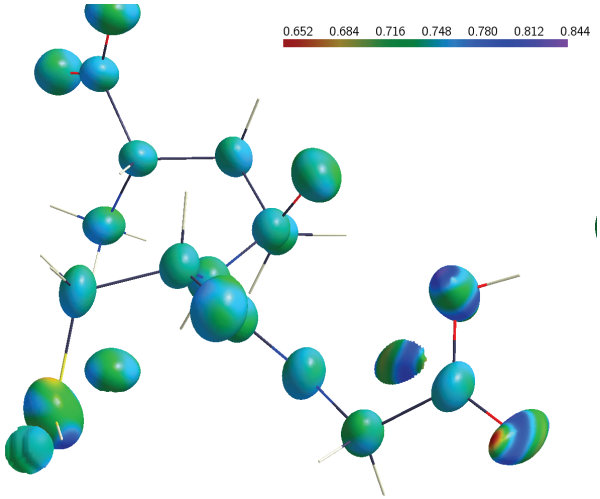

Figure 1. Isosurface of the MEM-electron density of Glutathion at 5 eÅ^{-3} mapped with the electron density value of the harmonic prior density. Atoms in green show almost no anharmonic effect.

Keywords: anharmonic motion, maximum-entropy-method, Glutathion

MS29. Quasi crystals and aperiodic materials

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MS29-P1 An Icosahedral Quasicrystal as a golden modification of the icosagrid and its connection to the E8 lattice

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We present an icosahedral quasicrystal as a modification of the icosagrid, a multigrid with 10 plane sets that arranged with icosahedral symmetry. We use the Fibonacci chain to space the planes obtaining a quasicrystal with icosahedral symmetry. It has a surprising correlation to the Elser-Sloane quasicrystal [4], a 4D cut-and-project of the E8 lattice. We call this quasicrystal the Fibonacci modified icosigrid quasicrystal(FMIQ). We found that the FMQC totally imbeds another quasicrystal that is a compound of 20 3D slices of the Elser-Sloane quasicrystal. The slices, which contains only regular tetrahedra, are put together by a certain 'golden rotation' [5]. Interesting 20Gs (20-tetrahedron clusters arranged with the 'golden rotation') appear repetitively in the FMQC and are arranged with icosahedral symmetry. It turns out that this 'golden rotation' is the dihedral angle of the 600-cell (the super-cell of the Elser-Sloane quasicrystal) and the angel between the tetrahedral facets in the E8 polytope known as the Gosset polytope. We suggest that the FMIQ is an alternative result of releasing the transdimensional "geometric frustration" while maintaining the regularity of the tetrahedra.

Keywords: icosagrid, Fibonacci, Elser-Sloane quasicrystal, E8, 600-cell