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Double-stranded DNA viruses infect Archae living in hot springs at temperature above 80 ℃ . They are radically different in their properties from viruses that infect Bacteria and Eukarya. Not only are the shapes of these viruses different to all other viruses found on Earth, but ca 90% of their putative genes do not have any homologs in other viruses or cellular life forms (1). Their ecological, morphological and genomic originality raises intriguing questions about their biology and their origins. Combination of electron microscopy and X-ray crystallography has revealed a nucleosome-like organization for the lipothrixvirus Acidianus Filamentous Virus 1 (AFV1) that has not been yet observed for any linear viruses. The three-dimensional reconstruction of AFV1 core has revealed a left-handed helical structure similar to those in the eukaryal nucleosome. In this architecture, one of the two major structural proteins, the basic ORF132 might form a histone-like central proteic core with the DNA super helix wrapped around. The second structural protein, ORF140, is located peripherically. We propose that its helical and elongated N-terminus, charged positively, is in contact with DNA, probably binding major grooves. The globular C-terminus domain contains an amphilic helix and harbours buried octyl-glucoside molecules. It might, together with associated lipids, form the outer coat of the virus. Structural characterizations of these fascinating DNA archaeal viruses, already described with the virus STIV (2), contribute to a recent upsurge of interest in the evolution of virus in general.

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Keywords: virus structure, X-ray macromolecular crystallography, electron microscopy

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Structural studies of Holliday junction resolvases from bacteriophages, archaea and yeast

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Holliday junctions (HJ) are central intermediates in repair and reorganization of DNA by homologous recombination. HJ-resolving enzymes (also known as HJ resolvases) mediate the resolution of the 4-way junction by introducing symmetrical nicks in opposing strands. Members of this ubiquitous family of structure-specific endonucleases function as dimers and require divalent cations for cleavage. We have previously reported the crystal structure of a HJ complex of Phage T4 endonuclease VII (EndoVII), an enzyme, which is involved in mismatch repair and the resolution of branch points prior to packaging of DNA into the phage head. The conformation of the EndoVII-bound HJ represents a hybrid between the standard stacked-X and square-planar conformations, demonstrating how the junction is recognized and distorted by an induced-fit mechanism. We have also solved the crystal structures of cruciform cutting enzyme 1 (Cce1) from Candida glabrata and of the HJ cutting enzyme (Hjc) from the hyperthermophile archaeon Archaeoglobus fulgidus at 3 and 1.7Å resolution, respectively. They represent two structurally distinct resolvase families with the same biological function, but exhibiting clearly different substrate specificities. Recently we have determined the structure of a HJ complex of A.fulgidus Hjc at 3.2Å resolution. Surprisingly, in this complex two Hjc dimers are bound to the junction, which exhibits an essentially undisturbed stacked-X conformation. Common features as well as striking differences in the mode of junction binding and recognition among the structurally characterized members of the resolvase family will be discussed.

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Keywords: Holliday junction resolvases, endonuclease VII, Hjc, Cce1, crystal structure

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Charge density based ligand design

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Recently we synthesised and experimentally determined the charge density in molecular species to gain insight in their reactivity and coordination behaviour. Not to judge on the structure-reactivity relationship by mere bond lengths comparison we rather relay on the topological analysis on the basis of high resolution data and a multipole refinement. Various topics are addressed in the talk:
S=N bonds in polyimidosulfit ylides are rather easy to cleave because they are electrostatically reinforced S+—N— single bonds rather than hetero-olefin bonds and the formal S=C double bond is a polar S+—C— single bond with no ylenic contribution;
The same is valid for P=N bonds. Reducing of iminophosphoranes to phosphanes is feasible under the right conditions, even though they are known to be thermodynamic sinks;
The metallaphosphane [Me2Al(mu-Py)2P] contains a divalent P(III) atom with two lone pairs at the central phosphorus atom. Following this finding the P-atom in the protonated phosphanide PPy2(H) can be employed in mu-bridging mimicking a 4-electron donor;
Multipole refinement of an alpha-lithiated benzyl silane provides insight in the electronic situation and thus the observed stereochemical course of transformations. Surprisingly the negative charge generated at the carbanion hardly couples into the phenyl ring;
The Laplacian distribution around the boron atom in [{$Cp(CO)_2Mn$}$_2$(mu-BtBu)] with its three VSCCs clearly shows the difference between the borylene ligand and the carbonyl ligand. The complex has to be classified as a dimetalloborane with no Mn-Mn bond rather than a borylene complex.

Keywords: ligand design, charge density studies, structure and function

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Non-linear optical properties & structure determination by combining X-ray data and QM wavefunctions

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