of molecular structures for $C_{70}Br_{10}$ or $C_{60}Cl_{24}$, which have been later confirmed by X-ray crystallography (partially with the use of synchrotron radiation). For the mixture of two compounds with known X-ray structures, $C_{60}Cl_{28}$ and $C_{60}Cl_{30}$, the experimental IR spectra were interpreted by comparison with the calculated ones using subtle differences for compounds possessing very similar structures. For the mixture of isomeric molecules in the same crystal (examples: $C_{70}Cl_{28}$ [1], $C_{60}F_{48}$, and $C_{78}Br_{18}$ [2]), theoretically predicted structures were helpful in the search for suitable disordering model in LS refinements.

Thus, simultaneous use of X-ray crystallography, IR spectroscopy, and theoretical calculations resulted in obtaining highly valuable structural information for many halogenated fullerenes.

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Keywords: fullerene halides, molecular structure, DFT

MS10.24.5

Acta Cryst. (2005). A**61**, C20

The Nature of the HB. 3. Towards a Comprehensive HB Theory

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Communications 1 and 2 have shown that the *empirical laws* governing HB strength can be reduced to two main points: (*i*) The PA/pK_a Equalization Principle; and (*ii*) The Six Chemical Leitmotifs. Much more difficult is the formulation of a *HB theory*, that is a complete explanation of the two empirical laws in terms of basic chemical bonding theory. Our method relies on what we have called *"The Transition-State HB Theory"* according to which any X-H…Y bond can be considered as a proton-transfer (PT) reaction X-H…Y ↔ X…H…Y ↔ X…H-Y which is bimolecular in both directions, proceeds *via* the X…H…Y transition state (the activated complex) and differs from ordinary reactions only because reactants and products are pre-bound by the HB, so that rather small PT-barriers are to be expected. This method is applied to the study of O-H…O and N-H…O/O-H…N RAHBs by quantum-mechanical DFT emulation with full geometry optimization of the three stationary points or of the complete PT-pathway profile. Analysis of the data was performed, in a VB logic frame, by the Marcus rate-equilibrium relationships, extrathermodynamic LFER Hammett parameters and avoided crossing (state correlation) diagrams. Results show that HB strength, single or double-well shape of the PT-pathway and height of the PT-barriers are completely determined, for any R_1X-H…YR_2 HB, by the ability of the R_1 and R_2 substituents to achieve the condition of PA/pK_a matching between the HB donor and acceptor molecules. The theory is used to interpret accurate variable-temperature X-ray crystallographic data.

Keywords: hydrogen bond theory, proton transfer, variable-temperature X-ray crystallography

MS11 INSTRUMENTATION AT NEXT GENERATION X-RAY SOURCES

Chairpersons: Thomas Tschentscher, John Arthur

MS11.24.1

Acta Cryst. (2005). A**61**, C20

Roles of X-ray Optics in the Next Generation X-ray Source

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X-ray optics for x-ray free-electron lasers (XFEL) are very important for beam handling/diagnostics, and, potentially, for FEL generation. In particular, special characters of XFEL such as high spatial coherence, short pulse, and peak brightness, should be well considered in the design work.

For beam handling (*i.e.,* monochromatization, focusing, filtering, *etc.*), conventional optical components are still important. However, higher qualities are required to avoid unwanted speckles under coherent illumination [1,2] and to keep high brightness. Diagnostics of coherence properties, temporal profile, and photon statistics [3] give crucial information for accelerator operation as well as for user applications. Shot-by-shot and non-destructive methods are highly desirable. X-ray monochromator is a key issue to realize a seeded XFEL such as the two-staged configuration [4].

In order to meet these severe requirements, several R&D programs utilizing presently available synchrotron sources are in progress. Achievements and current problems are discussed.

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Keywords: X-ray optics, free electron lasers, synchrotron X-ray instrumentation

MS11.24.2

Acta Cryst. (2005). A**61**, C20

Ultrafast X-ray Studies of Structural Dynamics

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The physical and chemical transformation of matter on the atomic scale typically occurs in many femtoseconds to a few picoseconds and involves the motion of atoms on the Ångström length scale. The unique capabilities of linac based light sources match the natural time and length scale of structural dynamics and provide scientists with an outstanding opportunity to better understand the chemical and physical transformations of matter. Results from the recently commissioned Sub-picosecond Pulse Source (SPPS) at the Stanford Linear Accelerator Center (SLAC) will be utilized to highlight the unique capabilities and challenges of linac based ultrafast light sources. The projected capabilities of the Linac Coherent Light Source (LCLS) and a brief description of the science it will enable will also be discussed.

Keywords: time-resolved structural studies, femtosecond X-ray sources, X-ray free electron lasers

MS11.24.3

Acta Cryst. (2005). A**61**, C20

Imaging of Single Molecules

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The path toward imaging single molecules with a free electron laser presents several challenges: from the particle injection and partial physical orientation to the ability to produce x-ray pulses that are short and intense. From short pulses required to the collection of the data with the appropriate detectors. From the classification of the orientation of millions of images to their phasing. Some of these problems will have to wait for the available sources, while others can be studied now by simulations or experiments. We will present some of these experiments, and discuss experimental requirements.

Keywords: non-crystallographic phase retrieval, biological molecules, instrumentation

MS11.24.4

Acta Cryst. (2005). A**61**, C20-C21

Parabolic Refractive X-ray Lenses

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Parabolic refractive x-ray lenses are novel optical components for the hard x-ray range from about 5 keV to about 120 keV. They are compact, robust, and easy to align and to operate. They can be used like glass lenses are used for visible light, the main difference being that the numerical aperture is much smaller than one (of order 10^{-3} to 10^{-4}) [1-3]. They have been developed at Aachen University and are made of aluminium and beryllium. Their main applications are in