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### CRYSTALLOGRAPHIC LESSONS AND FUNCTIONAL INSIGHTS FROM THE STRUCTURE OF THE 30S SUBUNIT

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The 30S ribosomal subunit is responsible for binding mRNA and the anticodon stem loop of tRNA. By monitoring codon-anticodon interactions in the decoding process, it greatly increases the fidelity of translation. Although the smaller of the two subunits, it has a molecular weight of almost a megadalton, and determination of its structure presented challenging problems in crystallization, data collection and phasing. We describe some general conclusions from the structure determination of the 30S ribosomal subunit. In particular, careful and extensive use of anomalous scattering was essential to obtaining useful high resolution phases. We also describe insights into the decoding mechanism from the structure of the 30S subunit complexed with antibiotics and mRNA and tRNA ligands. The 30S subunit discriminates between correct and incorrect tRNAs through an induced fit mechanism that closely monitors the minor groove geometry of base pairing at the first two positions of the codon-anticodon helix. These studies provide a structural rationale for the wobble hypothesis and why degeneracy in the genetic code is tolerated at the third position. They also show in structural terms how aminoglycoside antibiotics affect the fidelity of translation.

#### Keywords: RIBOSOME ANOMALOUS SCATTERING

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#### MOBILITY, FLEXIBILITY AND INHIBITION OF PEPTIDE BOND FORMATION

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The atomic structures of both ribosomal subunits from eubacteria, *Thermus thermophilus* and *Deinococcus radiodurans*, were determined under close to physiological conditions. The structures of their complexes with antibiotics, substrate analogues and cellular factors highlighted region of a high mobility, revealed the mechanisms of selected steps in protein biosynthesis, suggested how antibiotics may inhibit this process and illuminated elements that may confer selectivity for clinically relevant antibiotics.

Comparative studies indicated the flexibility of many functionally relevant features and showed that under less physiological conditions they may become disordered, as in the structure of the large subunit from *Haloarcula marismortui*. Among the flexible features is the perturbing arm that serves as the gate for the exiting tRNA, the region that hosts the GTPase activity, and intersubunit bridges that are formed upon the association of the two subunits.

Analysis of the binding modes of substrate analogues favors the suggestion that the peptidyl transferase center serves as a template for proper positioning of tRNAs rather than participating in catalytic events of peptide bond formation. This template may include a few ribosomal proteins, but it is largely made of RNA segments, including the intersubunit bridge connecting the peptidyl-transferase site in the large subunit and the decoding region in the small one. This bridge plays also a major role in positioning and orienting the tRNA molecules, and assists translocation of tRNA molecules between the Aand P- sites.

#### Keywords: RIBOSOME, TRNA, ANTIBIOTICS

## Acta Cryst. (2002). A58 (Supplement), C3 WHAT HIGH PRESSURE CAN DO FOR YOU?

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The science enabled by high-pressure research is experiencing an unprecedented surge of breakthroughs lately as technical limitations are lifted. Improved and versatile diamond anvil cells, large volume presses and brighter X-ray and neurons sources enable interdisciplinary teams to tackle new and long-standing issues. Crystallography is at the center of these developments. As with studies at ambient pressure conditions, it straddles disciplines and provides the necessary atomic level understanding to explain the phase transitions, new materials and novel properties that result when atoms and molecules occupy smaller volumes. For example, simultaneous measurements of elasticity and crystal structure under conditions of relevance to the Earth serve to test models for compositional and temperature variations of the planet. Following the time dependence of structure during phase transitions constrain those structural features most important in transformations. The origin of unexpected behaviors, such as pressure-induced expansion in corner-connected frameworks, can be traced to changes in crystal structure and in site preferences for water. Finally, iso-chemical decrease in volume leads to new materials, enhancement of dielectric properties over what is observed in the phase stable at ambient conditions, and to a means of studying non-bonding and H-bonding interactions with less ambiguity.

### Keywords: HIGH PRESSURE TIME RESOLVED ZEOLITES

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# NEW SUPERCONDUCTOR MgB<sub>2</sub> AND RELATED COMPOUNDS J. Akimitsu

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Last year, we have reported the two new boride-compounds; one is  $MgB_2$  - a new high  $T_c$  superconductor, another is  $CaB_2C_2$  - a new high-  $T_c$  ferromagnet. In this talk, I describe the present status for both systems, which might introduce to a new 'p electron physics'.