

MS47-P1 X-ray-induced overall structural changes in a protein molecule at cryogenic temperatures. Tatiana Petrova,^{1,2} Vladimir Y. Lunin,¹ Stephan Ginell,² Andre Mitschler,³ Youngchang Kim,² Grazyna Joachimiak,² Alexandra Cousido-Siah,³ Isabelle Hazemann,³ Alberto Podjarny,³ Krzysztof Lazarski,² and Andrzej Joachimiak² ¹*Institute of Mathematical Problems of Biology, Russian Academy of Sciences, Pushchino, 142290 Russia,* ²*Structural Biology Center, Biosciences Division, Argonne National Laboratory, Argonne, Illinois, 60439 USA,* ³*Département de Biologie Structurale et Génomique, IGBMC, CNRS, ULP,INSERM, 1 rue Laurent Fries, B.P. 163, 67404 Illkirch, France.*
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Radiation-induced structural changes in a protein molecule were studied in a series of diffraction experiments in which multiple data sets corresponding to increasing absorbed doses were collected from the same crystals of human aldose reductase (h-AR) and elastase at atomic resolution [1, 2]. It was found that irradiation causes the displacement of big parts of the protein molecule and water network. These structural changes have a cooperative character: big parts of protein molecules are displaced approximately as rigid bodies. Water molecules move in concert and in the same direction as adjacent protein atoms. There is a pronounced correlation between collective atomic movements and local and global damage to the crystal. Radiation-induced atomic shifts start at places with the pronounced local damage and are the largest for the damaged residues and structure fragments connected to damaged residues. The displacement of secondary structure elements leads to the expansion of the protein globule, which occurs synchronously with, and in the same direction as, the expansion of the unit cell. Radiation-induced structural changes at 100 and 15K were studied. The data at different temperatures were collected from different parts of one and the same crystal. It was found that lowering the temperature from 100 to 15K decreases the disulfide-bond deterioration and atomic displacements, the decrease being somewhat greater than twofold. Concerning the global damage in the same experiment, lowering the temperature from 100 to 15K, allowed one to collect data of a high resolution limit of 1.55 Å instead of 1.75 Å. A possible interrelation between site-specific and global crystal damage, mediated by radiation-induced atomic displacements is discussed. Local and overall structural changes induced by radiation were compared with those induced by heating. A comparison of the models of h-AR and elastase at different temperatures shows that, in the case of temperature increase, the molecule expands mostly due to the movement of protruding loops and helices on the surface of the molecule. In the case of irradiation, along with the movement of loops and helices on the surface, the movement of big structural segments, including residues of inner beta sheets occurs. The difference is due to the fact that, during irradiation, some protein residues and crucial bonds between secondary structure elements are deteriorated, which facilitates the divergence of secondary structure elements, while in the case of temperature increase these bonds remain unchanged. A comparison of the increase in atomic displacement parameters caused by temperature and by irradiation suggests that, during irradiation, some side chain residues in the inner part of the protein molecule acquire multiple conformations.

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MS49-P1 Symmetry groups in moroccan geometric patterns achieved on wood. Youssef Aboufadi, Abdelmalek Thalal, Jamal Benatia, Abdelaziz Jali, My Ahmed Elidrissi Raghni, *Department of physics, LSM, Faculty of Sciences- Semlalia-Marrakech-Morocco*
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Different methods are used in Islamic ornamental art to draw geometric patterns. These methods depend on material support such as tiles, bricks, wood, brass, and plaster. Master craftsmen working on wood use a method called "Hasba" (unit measure). It consists in tracing within a square frame a P4m grid. Several patterns with the same symmetry may be generated from the underlying grid [1, 2]. P4m is the most encountered group in the moroccan geometric patterns. In this work we generalize the method to the other wallpaper groups as P6mm, C2mm, P4gm... We show that we may obtain new symmetries by acting on the P4m basic grid. Indeed if we add or remove some lines on the basic grid we change its symmetry and consequently the symmetry of constructed patterns (Fig.1-a). Furthermore it is possible to find symmetry other than P4m, by choosing a particular area of the P4m basic pattern and applying the 17 symmetry groups of the plan; this area is considered as the fundamental region of the new pattern (Fig.1-b).

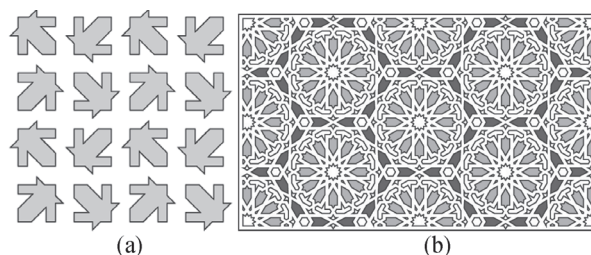


Figure 1: Patterns with symmetry group: a) P4gm, b) P6mm.

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