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EPR, Endor and DFT Studies on X-Irradiated Single Crystals of L-Lysine HCl $2H_2O$ and L-Arginine HCl H_2O YIYING ZHOU, WILLIAM H. NELSON — When proteins and DNA interact, arginine and lysine are the two amino acids most often in close contact with the DNA. In order to understand the radiation damage to DNA in vivo, which is always associated with protein, it is important to learn the radiation chemistry of arginine and lysine independently, and then complexed to DNA. This work studied X-irradiated single crystals of L-lysine·HCl·$2H_2O$ and L-arginine·HCl·H_2O with EPR, ENDOR techniques and DFT calculations. In both crystal types irradiated at 66K, the carboxyl anion radical and the decarboxylation radical were identified. Specifically, the calculations performed on the cluster models for the carboxyl anion radicals reproduced the proton transfers to the carboxyl group from the neighboring molecules through the hydrogen bonds. Moreover, computations supported the identification of one radical type within irradiated arginine as the guanidyl radical anion with an electron trapped by the guanidyl group. Based on the radicals detected in the crystal irradiated at 66K and at 298K, and the annealing experiments from the irradiation at 66K, the mechanisms of the irradiation damage on lysine and arginine were proposed, and the possible effects of irradiated arginine and lysine to the DNA within chromatin were analyzed.

Yiying Zhou
Georgia State University

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