Institut Ruđer Bošković

CIII. Kolokvij Zavoda za organsku kemiju i biokemiju i

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Professor Robert GLASER
Department of Chemistry,
Ben-Gurion University of the Negev, Beer-Sheva 84105, and
Feinberg Graduate School, Weizmann Institute o f Science, Israel.

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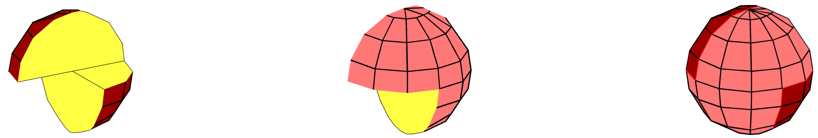
CHIRAL APPLE HALVES AS STRUCTURAL MODELS OF DOUBLE-HELICAL PARALLEL CHAINS



All the basic concepts and terminology of symmetry and extended arrays (e.g. unit-cells, asymmetric units, helical stereochemistry) will be explained in the introduction since audiences are usually unfamiliar with crystallographic nomenclature. The 'Royal Cut' (Coupe du Roi) represents an esthetic way used by some people to bisection apples into two homochiral identical halves. It can also be applied to rotational symmetry objects such as cubes, cylinders, cones, etc. The corresponding trisection affords three identical homochiral apple-thirds. It will be shown that Coupe du Roi cut apples represent a 4_2–screw rotation-symmetry double-helix repeat unit (unit cell) of intertwined homochiral identical halves. Of the eight symmetry operations, screw rotation (combined rotation and translation) is unique in that it is the only one that has its own right- or left-handed n_1 or n_{n-1}-screw-symmetry chiral pathways that are *independent* of the handedness of the individual molecules or polymeric residues that constitute the extended array in a crystal. For example, note the antiparallel right-handed poly(dA-dT)•poly(dA-dT) B-DNA duplex versus the $(dC\text{-}dG)_3$•$(dC\text{-}dG)_3$ left-handed Z-DNA duplex hexameric unit. On the other hand, $2n_n$–screw symmetry (2_1, 4_2, 6_3) arrangements do not have chiral pathways when they represent the spatial arrangement of individual molecules packed in a crystal. However, within Coupe du Roi bisected apples, the two remaining non-contiguous (separated) uncut horizontal ¼-arcs provide physical constraints (*i.e.* non-symmetry constraints) which induce chirality to a 4_2 double-helix depending upon the tropicity (directionality) of the cuts. Inspection of Coupe du Roi apples show that this non-crystallographic chirality affords a ½-turn double-helix composed of either two 4_1 right- or two 4_3 left-handed intertwined parallel strands. Ordinary single or multiple-helices require repeat units (unit cells) containing full-turns of a strand. The ability of a 4_2-unit cell to contain only a ½-turn of the duplex results from the cell's C_2-symmetry formula unit (either a top or bottom layer of two cut apple side-by-side quarters) occupying the $P4_2$ space group's 'special position of 2-fold rotational symmetry' since both C_2 axes spatially coincide. The result is a shrinking of the unit-cell's screw-axis from one-full turn to a length of only 1/2-turn. X-ray fiber diffraction of Poly(rA)•Poly(rA) acid form shows a unit cell of one ½-turn of a dextrorotatory 4_2 duplex composed of two intertwined parallel tetranucleotide units. The (*P*)-chirality of this arrangement results from the chemical constraint of having rA residues ligated (bonded) together into a polymeric strand (*i.e.* another non-crystallographic constraint). The chemical equivalent of a Coupe du Roi 6_3-symmetry trisectioned apple is the 1/3-turn fiber diffraction unit cell of a (1→3)-β-D-glucan Curdlan parallel triple-helix.