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# Abstracts of Forthcoming Articles

*Solid State Chemistry of Organic Polyvalent Iodine Compounds. V. The Crystal Structures of 3-oxo-3H-2, 1-benzoxiodol-1-yl* o*-bromobenzoate (Two Polymorphs) and 3-oxo-3H-2, 1-benzoxiodol-1-yl* o*-chlorobenzoate.* J. Zanos Gougoutas and D. G. Naae. Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455. Single crystal transformations of 2-iodo-2′-bromo-, and 2-iodo-2′-chlorodibenzoyl peroxides (*IIa* and *IIb*) yield topotactically aligned crystal structures of their respective isomers: 3-oxo-3H-2, 1-benzoxiodol-1-yl *o*-bromobenzoate (*Ia*) and its *o*-chlorobenzoate analog (*Ib*). Two of the polymorphic forms of *Ia* ($C_{14}H_8IBrO_4$) which are formed in crystalline *IIa* can also be obtained by crystallizing *Ia* from various solvents: (*Ia*–$\beta$), $a = 7.474$, $b = 13.994$, $c = 13.152$ Å, $\beta = 102.4°$, $Z = 4$, $P2_1/a$, and a disordered acicular form (*Ia*–$\alpha$) which appears to be orthorhombic, $a = 3.99$, $b = 26.553$, $c = 26.008$, $Z = 8$ ($Pbc2_1$ ?). The only form of *Ib* ($C_{14}H_8IClO_4$) obtained by crystallizations from solvents is also formed in crystalline *Ib*. The crystal structures of the isostructural *Ia*–$\beta$ and *Ib* have been determined but only the latter has been refined. ($R = 0.059$ for 2085 "observed" intensities.) The derivative crystal structure of *Ia*–$\alpha$ has been determined only in (100) projection ($R = 0.08$ for 156 observed intensities). The three structures contain similar chains of bimolecular units or "dimers." The "dimers" are analogous to those found in crystal structures of the benzoate, *m*-chlorobenzoate, *o*-iodobenzoate, and *o*-fluorobenzoate analogs of I. Novel polymorphs ($X_a$ and $X_b$) of *Ia* and *Ib* are formed during the solid state peroxide isomerizations. The isostructural $X_a$ and $X_b$ consist of chains of "dimers" which are similar to those in *Ia* and *Ib*.

*Solid State Chemistry of Organic Polyvalent Iodine Compounds. VI. The Crystal Structure and Topotactic Hydrolysis of 3-oxo-3H-2, 1-benzoxiodol-1-yl* o*-fluorobenzoate.* J. Zanos Gougoutas, Kuo H. Chang, and M. C. Etter. Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455. The compound 3-oxo-3H-2, 1-benzoxiodol-1-yl *o*-fluorobenzoate (*IIIc*) is formed as a topotactically aligned crystal structure when single crystals of its dibenzoyl peroxide isomer thermally decompose at room temperature. Independently it has been found that single crystals of *IIIc* grown from solvents are hydrolyzed to *o*-iodosobenzoic acid, *II*, and *o*-fluorobenzoic acid after ~4 weeks in a moist atmosphere at ~45°C. *II* is formed topotactically in a conservatively twinned arrangement in which the (100) planes of the equally present twin members are parallel to (001) of *IIIc*. In addition, the 4 Å *b*-axes of the twin members align with the 4 Å *a*-axis of *IIIc*. Other examples of topotactic hydrolyses resulting in twinned arrangements of *II* are cited in reference to the novel possibility that the favored mode of alignment (the specific topotaxy between the reactant and *one* twin member) is one which, when augmented by conservative twinning, results in a favorable interphase between the conservatively twinned members. The transformation *IIIc* → *II* and more than 20 other corroborating examples of topotaxy in our studies lead us to expect the alignment of 4 Å axes whenever they are present in both the reactant and product of topotactic transformations involving comparable aromatic molecules. The crystal structure of *IIIc* ($C_{14}H_8IFO_4$), $a = 4.08$, $b = 12.00$, $c = 26.25$ Å, $\beta = 90.5°$, $Z = 4$, $P2_1/c$ (refined to $R = 0.10$ for 453 photographically recorded intensities) consists of chains of *transoid* "dimers" similar to those previously observed in structures of closely related derivatives.

*$Ba_{15}Fe_7S_{25}$ and $Ba_3FeS_5$: Crystal Structures, Mössbauer, Magnetic and Electrical Behavior.* J. T. Lemley, J. M. Jenks, J. T. Hoggins, Z. Eliezer, and H. Steinfink. Department of Chemical Engineering, The University of Texas, Austin, Texas 78712. $Ba_{15}Fe_7S_{25}$ is prepared by reacting stoichiometric amounts of BaS, Fe, and S in evacuated quartz ampoules while $Ba_3FeS_5$ is obtained in a tetrahedral press at 50 kbar and 1000°C. The crystal structure of $Ba_{15}Fe_7S_{25}$ has been determined using 4053 independent, nonzero X-ray reflections measured by a counter technique. The compound crystallizes in the orthorhombic system, $Pnma$, $a = 41.91(1)$ Å, $b = 9.572(3)$ Å, $c = 12.654(3)$ Å, $\rho_{calc} = 4.14$ g/cc, $z = 4$. In both compounds, Fe is tetrahedrally coordinated to S, and Ba is in either