deformed specimens. As heating time increases the alloys were hardened and then softening again. This phenomena was explained by age-hardening and over aging. Lattice distirtion, which is associated with hardening, were confirmed by X-ray diffraction analysis. The Δa values were calculated taken the lattice parameter, a, at 3 minutes as origin. The measurement of lattice parameters showed a good correlaton with the hardness results. Lattice distortion was firstly decreased in the recrystallisation stage and then was increased as the age-hardening process began. Over aging leads to decreas in lattice distortion due to disappearance of the coherent strains. It can be concluded that during heat treatment of highly deformed Sn-Pb alloys the following processes take place : (a) sotening (recrystallisation), (b) hardening (age-hardening) and (c) softening (over aging). Therefore, high plastic deformation instead of quenching may influence the mutual interaction between the solid-state reactions during the subsequent heat treatment.

04.5–1   INTERMOLECULAR TRANSITION DIPOLE-DIPOLE COUPLING BETWEEN THE NON-CYANIDE LIGANDS IN SOME CRYSTALLINE PENTACYANO-L-METALLATES. By O.E. Piro and, in part, S.R. González and P.J. Aymonino, Depts of Physics and Chemistry, Faculty of Exact Sciences, National Univ. of La Plata, C.C.67, 1900 La Plata, R. Argentina.

The nature and magnitude of intermolecular vibrational coupling of NO groups in $Sr[Fe(CN)_5NO]$ $.4H_2O$ and $Ba[Fe(CN)_5NO].2H_2O$ and of the antisymmetric stretching mode of N_3 ligands in $K_3[Co(CN)_5N_3].2H_2O$ were studied on the basis of reported crystallographic and spectroscopic data. In all three compounds, the non-cyanide ligands of the complex ions are piled up in an antiparallel quasi-eclipsed fashion at distances of about 4 Å, forming linear chains in the crystals. The fine structure of the NO stretching band in the IR spectra of polycrystalline $Sr[Fe(CN)_5N(^{16}O/^{18}O)].4H_2O$ isotopic mixtures and of single crystals of $Ba[Fe(CN)_5NO].2H_2O$ can be interpreted in terms of a linear-chain model of $[Fe(CN)_5NO]^{2-}$ ions coupled through their NO ligands via transition dipole-dipole forces. By this model, the value $|(\partial m/\partial S)_0|=13$ Debye/Å is obtained for the NO dipole-moment derivative and $f_1=0.172$ and the average $\bar{f}_1=0.189$ mdyne/Å values for the force constants that respectively couple the NO stretching vibration in the barium and strontium salts. Similar calculations for $K_3[Co(CN)_5N_3].2H_2O$ ($S.G.P\bar{1}$) explain the Davydov splitting of 25 ± 2 cm^{-1} observed in the frecuencies of the IR- and Raman-active vibrations associated with the N_3 antisymmetric stretching mode. The value $|(\partial \mu/\partial Q_3)_0|=263$ (esu)/gr$^{1/2}$ was obtained for the dipole-moment derivative of this mode, and the value $f_3=0.071$ mdyne/Å for the force constant that couples such vibrations in the crystal.

04.5–2   CRYSTAL STRUCTURES OF PERMETHYLATED α-CYCLO-DEXTRIN COMPLEXES WITH L- AND D-MANDELIC ACIDS By K. Harata, Research Institute for Polymers and Textiles, 1-1-4 Yatabe-Higashi, Tsukuba, Ibaraki 305, Japan; K. Uekama, M. Otagiri, and F. Hirayama, Faculty of Pharmaceutical Sciences, Kumamoto University, 5-1 Oe-honmachi Kumamoto 862, Japan.

Cyclodextrins form diastereoisomers by including optically active guests within the cavity of the macrocyclic ring. Permethylated cyclodextrins are expected to have higher stereo-selectivity in the complex formation with chiral guests because of the distorted conformation of the macrocyclic ring. The crystal structures of permethylated α-cyclodextrin (methyl-α-CDx) complexes with L- and D-mandelic acids (L-MA and D-MA, respectively) are reported, and the chiral recognition in the crystalline state is demonstrated.

The methyl-α-CDx complexes with L- and D-mandelic acids crystallized in the space group $P2_1$ with the following crystal data: (1) L-MA complex, $C_{54}H_{96}O_{30} \cdot C_8H_8O_3 \cdot 3H_2O$, F.W.=1431.5, a=13.123(2), b=23.187(4), c=13.113(2) Å, β=107.19(1)°, D_x=1.247 g·cm^{-3}; (2) D-MA complex, $C_{54}H_{96}O_{30} \cdot C_8H_8O_3 \cdot 2H_2O$, F.W.=1413.5, a=11.624(2), b=23.739(4), c=13.786(2) Å, β=106.56(1)°, D_x=1.289 g·cm^{-3}. The structures of the above complexes were solved by the trial-and-error method combined with the rigid-body least-squares technique and refined by the block-diagonal least-squares method to the R-values of 0.087 for 4837 reflections (L-MA complex) and 0.055 for 4925 reflections (D-MA complex).

As shown in Fig. 1A, the methyl-α-CDx molecule of the L-MA complex has a pseudo two-fold symmetry. A water molecule is included at the O(6) side of the cavity, and links two glucose residues facing each other by the O(6) ···water···O(6) hydrogen-bond bridge. The phenyl group of L-MA is partly included at the O(2), O(3) side of the methyl-α-CDx ring, while the hydroxyl and carboxyl groups, protruding outside the cavity, form hydrogen bonds with water molecules. The methyl-α-CDx molecule of the D-MA complex is distorted so as to include tightly the phenyl group of D-MA (Fig. 1B). The O(6) side of the cavity is capped by an O(6)CH$_3$ methoxy group. The hydroxyl group of D-MA is hydrogen-bonded to an O(2) oxygen atom of methyl-α-CDx, while the carboxyl group forms the hydrogen bond with an O(6) oxygen atom of the adjacent methyl-α-CDx molecule. Therefore, methyl-α-CDx binds the D-MA molecule more strongly through the induced-fit type conformational change and the host-guest hydrogen bond.

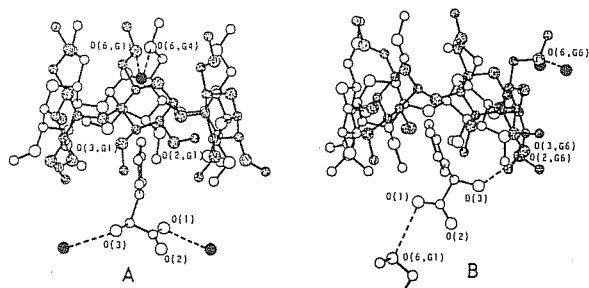Fig. 1. The inclusion feature of the methyl-α-CDx complexes with L-MA (A) and D-MA (B). Water molecules are shown by full circles.