

MS22-P1 *Ab initio* structure analysis of hexagonal MnO using X-ray powder diffraction data Yong-il Kim,^a Ki min Nam,^b Joon taik Park,^b ^aKorea Research Institute of Standards and Sciece, South Korea, ^bDepartment of Chemistry, Korea Advanced Institute of Science and Technology, South Korea
E-mail: yikim@kriss.re.kr

Most transition metal oxides have a cubic rocksalt crystal structure, but ZnO and CoO are the only stable transition metal oxides known to possess a hexagonal structure. The synthesis of hexagonal manganese oxide (h-MnO) is unprecedented thus far, although the theoretical calculations for the hypothetical h-MnO compound suggest various potential applications such as conventional sensors, actuators, energy storage devices and so on. In this respect, we tried to synthesize h-MnO and to do the *ab initio* crystal structure determination of the synthesized manganese oxide on the carbon sphere substrate from thermal decomposition of a single precursor, manganese acetylacetonate [Mn(acac)₂], in benzylamine. To determine the crystal structural information of the synthesized material, the single line fitting technique of the total pattern analysis solution program was used to extract the contribution of the crystalline phase from the diffraction pattern [1]. Preliminary indexing of the diffraction pattern was performed using the pattern decomposition method [2], and the pattern was finally indexed by the space group assigned as *P6₃mc*. A subsequent Le Bail profile fit was performed to extract the diffraction intensities and to refine the unit-cell parameters. The extracted intensities were used in the direct method for the structure determination [3]. The model determined using the direct method was refined by the Rietveld method [4, 5]. The final converged weighted *R* factor (*R*_{wp}) and the goodness-of-fit indicator [*S* (= *R*_{wp}/*R*_e)] were 4.17 % and 1.18, respectively. The crystal structure of the synthesized MnO was a member of the hexagonal crystal system and consists of tetrahedrally coordinated Mn and O atoms. The selected interatomic distances of hexagonal MnO have a short axial bond of 1.9630(4) Å and three longer equatorial bonds of 2.0790(4) Å with a ratio of 0.944. The bonding angles of O-Mn-O in a tetrahedral coordination by oxygen are 110.549(6) and 108.372(6), respectively.

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MS23-P1 Structural relations between particular and double brucinium diastereomeric salts. Agata Białońska, Zbigniew Ciunik, Faculty of Chemistry, University of Wrocław, Poland
E-mail: agata.bialonska@chem.uni.wroc.pl

For many reasons, fractional crystallization of diastereomeric salts remains one of the most frequently used methods for a separation of racemic acids/bases into their chiral components [1]. Besides particular diastereomeric salt crystallizing fractionally, an attempt to separate racemate into its chiral components by the method may lead to precipitation of a solid solution of both diastereomeric salts, characterized by changeable ratio of particular salts. Diastereomeric salts can also form crystals of double salts with fixed stoichiometric ratio of both. While differences in crystal structures of particular diastereomeric salts usually lead to their fractional crystallization, great similarities in their crystal structures may lead to formation of solid solutions. However, there is no a rule based on similarities/differences of particular diastereomeric salts which could point at reasons of diastereomeric double salt formation. An attempt to separate some racemic *N*-(3,5-dinitrobenzoyl)-amino acids by fractional crystallization of brucinium diastereomeric salts leads to crystallization of diastereomeric double salts. Among these derivatives, there are *N*-(3,5-dinitrobenzoyl)-DL-alanine and *N*-(3,5-dinitrobenzoyl)-DL-serine. Crystallization of particular brucinium diastereomeric salts, ones containing D- and others containing L-enantiomer of the alanine or the serine derivative leads to interesting results. In most of the cases high *Z'* structures were obtained, and among them unique *Z'* = 14 structure. In other cases the brucinium salts cocrystallize with molecular brucine or *N*-(3,5-dinitrobenzoyl)-amino acid.

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