FIBRE BUNDLE APPROACH TO THE DERIVATION OF THE ENERGY FUNCTIONAL OF A PHYSICAL SYSTEM WHOSE SYMMETRY IS DESCRIBED BY A EUCLIDEAN GROUP

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The fibre bundle formalism has been applied both to the symmetry groups of a physical system and to the energy functional itself. As a result of this procedure additional terms in the energy functional responsible for the symmetries of a physical system have been derived. The explicit form of these terms has been found in the case when the corresponding symmetry group is a rotation group $SO(n)$, a translation group T_n and a Euclidean group which is their semi-direct product. In the case of the discrete subgroups of the Euclidean group (i.e. in the case of the crystallographic groups) the well-known conditions on the potential part in the energy functional have been obtained.

Keywords: FIBRE BUNDLES, ENERGY FUNCTIONAL, EUCLIDEAN GROUP

POTENTIAL PITFALLS IN DATA COLLECTION AND SPACE GROUP ASSIGNEMENT

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Determination of the correct space group is an important first step in any crystal structure determination. Ambiguities in space group selection arising due to lattice pseudo-symmetry, inconsistencies in systematic extinctions, and inconclusive E statistics comprise a source of errors that may lead to incorrect space group assignment and flawed structures. While personal experience and software programs such as CHECKCIF and PLATON can be used for space group verification, caution must be exercised in the usage of such programs and the resulting effects on the crystals structure interpretation.

For instance, in the structure of $[Hpy][NbOCl_4(py)].(py)$ (py = pyridine), an analysis of intensities of hkl reflections with k+l odd and examination of the molecular symmetry indicated that the correct space group was *Pnc*2.

However, programs PLATON, CHECKCIF, and FINDSYMM all suggested space group *Amm*2 instead of *Pnc*2, while XPREP indicated *Pnc*2, a subgroup of *Amm*2. Weak data present another recurrent problem nowadays as smaller crystals of inferior quality are being analyzed with highly sensitive area detector diffractometers. The weakness of data may leads to wishful structure extrication, especially when the data quality is not sufficient to provide adequate atomic resolution and systematic absence recognition is severely hampered. These pitfalls are discussed and illustrated with examples.

Keywords: SPACE GROUP ASSIGNEMENT, PSEUDO-SYMMETRY, SOFTWARE

PECULIARITIES OF RESOLVING OF CRYSTAL STRUCTURES OF ORGANIC METALS AND FULLERENE COMPOUNDS

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The alternation of anionic and cationic layers is characteristic feature of crystal structures of cation-radical salts with high electroconductivity (organic metals). Often symmetry of these layers differs, moreover, they can be described in different space group, that results in difficulties at resolving of crystal structures. We detected the pseudo-symmetry in many organic metals (for example, α-$(BETS)_6Bi_3Cl_{12}(PhCl)$, k-$(BETS)_4Cu_3Cl_8$ [BETS = bis(ethylenedithio)tetrathiafulvalene]). It has been earlier revealed, that the pseudo-symmetry is characteristic for some crystal structures of fullerenes. Despite of external similarity, C_{60} and C_{70} with same reagents frequently do not form isostructural compounds. We have carried out the X-ray study of C_{60}-$2[(Ph_3P)AuCl]$ (1) and C_{70}·$2[(Ph_3P)AuCl]$ (2). The crystal structures of these complexes are characterized of trigonal and monoclinic symmetry accordingly. Besides the pseudo-symmetry also was found out in complex 2. Positions of $[(Ph_3P)AuCl]$ molecules correspond to *C*2/*m* space group, while the C_{70} molecule has no the centre of symmetry, and consequently its position can be described only in *Cm* space group. Taking into account the possible pseudo-symmetry can simplify the resolving of crystal structures of organic metals and fullerenes.

Keywords: PSEUDO-SYMMETRY , ORGANIC METALS, FULLERENES

TABLES OF MAGNETIC SPACE GROUPS

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Properties of the magnetic space groups are tabulated in a format and content similar to that of the International Tables of Crystallography. For each group we have tabulated: diagrams of symmetry elements; diagrams of general positions origin; asymmetric unit; symmetry operations; generators selected general and special positions; and symmetry of special projections

The symmetry operations are given in the traditional International Tables notation and in Seitz notation. The magnetic moments allowed by magnetic symmetry are given in the diagrams of general positions and the listing of general and special positions.

Keywords: MAGNETIC SPACE GROUPS, SYMMETRY, GROUPS