Angular parts of one-electron wave functions are simulated by linear combinations of spherical harmonics transformed on irreducible representations of point groups (solid or Cartesian harmonics). So each symmetrical association of electrons accompanies with the same radial orbital. Even use of one-determinant many-electron wave function permits to take into account a part of correlation energy.

Central ion orbitals are orthogonalized to ligand ones with the help of Lagrange multipliers by original procedure. In consequence, the contribution of ligand potential to self consistent field equations gets simplified. The expression for external potential field at the central d-metal ion was generated from Slater Type Orbitals of ligands. In order to simulate the environment of ligands in crystals a very simple physical model "ions in crystal" (E. Paschalis, A. Weiss, Theor. Chim. Acta, 1969, 13, 381) was used. This means that ligand is embedded in a hollow charged sphere with radius approximately equal to metal-ligand bond distance.

We have programmed DODAF formalism and applied it to several model systems such as Ni^{2+}/ZnO, Ni^{2+}/MgO, Cu^{2+}/CdO with satisfactory results. HF equations for transition metal ions were solved numerically (self consistency was reached up to 10^{-9}).

Some numerical aspects, especially the convergency properties of this method with respect to the number of ligands, their electronic structure and particular geometry, are discussed.

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SOME PRINCIPLES AND RESULTS OF HT-SUPERCONDUCTOR LIKE STRUCTURES DESIGN.

By S. F. Solodovnikov*. Russian Academy of Sciences, Siberian Pranch, Institute of Inorganic Chemistry, Novosibirsk, Russia.

The crystal structures of cuprate super-conductors and related compounds (more than 70 structure types) were analysed. The structures may be considered as sequences of plane square atomic nets of 9 types, 5 types of which being realized in HTSC structures. Based on the net approach to crystal chemistry and modelling of HTSC-related structures their maximum symmetry was shown to be within framework of 10 space groups: I4/mmm, P4/mmm, P4/nmm, P4mm, Immm, Ammm, Bmmb, Bmm2, Pmmm, and Pmmb. Proceeding from the building principles analysis of revealed HTSC structure types, empiric selection rules of the most probable structure models were formulated. Practically such sturctures contain no more than two different perovskite-like (involving copper-oxygen sheets) or additional (rock salt-, fluorite-type etc.) blocks with multiplicity for each of the blocks no more than three single sheets. Exceptions from this rule seem to be cuprates with only rock salt-type blocks which can include perovskite-like blocks with up to 6 copper layers, however, here again preparation of more than triple copper-layer compounds is rather complicated. Fluorite-like blocks in HTSC-related structures were assumed to be single because cuprates with a higher multiplicity of this block are not superconducting. It was also taken into account a rule of thumb that in mixed-layer compounds with different blocks of the same type (e. g. rock salt-type) their multiplicities may differ only by 1.

Using the formulated rules (some details for brevity omitted) the most probable models of HTSC-related structures were constructed. The total number of the models proved to be restricted to 73 variants (see Table), the biggest of which has 38 atomic nets in the unit cell corresponding to the " c" parameter value of 7. 5 nm.

Table. Amounts of HTSC-like structures (N_i) vs net number (n) in unit cell

N_i / n	N_1	N_2	N_3	N_i / n	N_1	N_2	N_3
2	1	1	1	20	2	—	—
4	1	1	1	22	5	1	1
6	5	5	5	24	0	—	—
7	1	1	1	26	9	1	1
8	5	4	3	28	1	—	—
9	2	2	1	30	3	—	—
10	5	4	3	32	0	—	—
12	6	2	1	34	4	1	1
14	9	5	5	36	0	—	—
16	6	3	3	38	1	—	—
18	7	2	2	total	73	33	29

Notations: N_1—the most probable models
N_2—HTSC-related cuprates
N_3—cuprate superconductors

PS-09.01.13 ENUMERATION AND IDENTIFICATION OF CRYSTAL-STRUCTURE TYPES BY A COMPUTER. By Masahiko HOSOYA* and Keiichirou TAKUSHI, Department of Physics, University of the Ryukyus, Japan

A computer program is presented to enumerate and identify crystal-structure types. If a chemical formula of contents in a primitive cell is given, the program enumerate all the possible structures for every space group, each of which is specified by the detailed arrangement of the atoms in the cell. Conversely, if a way of arrangement of the atoms is given, the legal name of the structure can be obtained uniquely in the present nomenclature. So any structure can be identified with another according to whether their names are reduced to the same legal one or not.

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Example

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Consider an intermediate step of the structure analysis of KH2PO4. If the space group and the number of molecules in the primitive cell have been obtained, the program can answer all the possible types as far as the symmetry concerns. In the present case, the space group is I42d(122), and the number of molecules in the cell is 2. First, the program requires the input of a genus. Input

A2B2C4D8

into the blank of a genus. It is given as follows.

KH2PO4 -> K2H4P2O8 -> K2P2H4O8 -> A2B2C4D8

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All the suffixes of the chemical formula should be doubled because two molecules are contained in a primitive cell. (We use letters of normal size for the suffixes for convenience of input.) Then the atomic symbols are arranged in increasing order of their suffixes. The Alphabet letters are substituted into each atomic symbol from A to Z. (It is indefinite whether A=K and B=P or A=P and B=K.) Such a sequence is called a genus. Input

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into the item of a space group, which is the number given in the International Table for Crystallography. The following seven answers will be given.

5:a2b2c4c4d4, 5:a2b2c4d4d4, 6:a2b2c4e8,
5:a2b2d4c4c4, 5:a2b2d4c4d4, 5:a2b2d4d4d4,
6:a2b2d4e8.

As an example, take the first one.

5:a2b2c4c4d4

The number 5 represents the degree of freedom that is the number of parameters which can be chosen freely. Letters after the colon show the atomic sites by the Wyckoff symbols. The correspondence between the atoms and the sites is as follows.

A2 B2 C4 D8
↓ ↓ ↓ ↓
a2 b2 c4 c4 d4

That is, atoms A, B, C are located at sites a, b, c respectively, while the eight D atoms are divided into two sets, one of which corresponds to c, the other to d.