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-electron ion was generated from Slater Type Orbitals of ligands. In order to simulate the environment of ligands in crystals a very simple physical model "ion in crystal" (E. Paschalis, A. Weiss, Theor. Chim. Acta, 1990, 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^{-n}).

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

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

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The crystal structures of cuprate superconductors and related compounds (more than 70 structure types) were analyzed. 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 modeling of HTSC-related structures their maximum symmetry was shown to be within framework of 10 space groups, 14/mmm, P4/mmm, P4/nmm, Pmmm, Amm2, Pnam, Pnnm, and Pnab. Proceeding from the building principles analysis of revealed HTSC structure types, empirical selection rules of the most probable structure models were formulated. Practically such structures 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 three copper-layer compounds in rather complicated. Fluorite-like blocks in HTSC-related structures were assumed to be single hexagonal 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.

**Example**

Consider an intermediate step of the structure analysis of KFePO4. If the space group and the number of molecules in the primitive cell have been obtained, the program can assign all the possible types as far as the symmetry concerns. In the present case, the space group is 142d(122), and the number of molecules in the cell is 2. First, the program requires the input of a genus. Input A2B2C4D into the blank of a genus. It is given as follows:

KFePO4 \rightarrow K2FePO4 \rightarrow K2Fe2(PO4)2 \rightarrow A2B2C4D.