Apatites form an extremely broad group of minerals. Due to the availability of numerous ionic substitutions, their reach varieties of composition allow for significant participation and role in many biochemical, petrologic, geochemical, engineering, and environmental processes. Despite constant intensive research and interest in apatites, the basic thermodynamic data for majority of the members of this group and related compounds are still lacking. **In this project, a new method for precise prediction of thermodynamic functions of state for apatites (enthalpy of formation, ΔH^o_f, Gibbs free energy of formation ΔG^o_f, entropy of formation S^o_f, heat capacity of formation ΔC^o_{pf}) is proposed for development and testing.** If confirmed, this will not only introduce numerous new data, but this novel approach might be in the future applied for other mineral groups and chemical compounds. Two major scientific hypotheses will be tested:

Hypothesis 1: There is strong correlation between thermodynamic functions of state and other, selected parameters (properties) of apatites and their components (e.g. electronegativity of ions, thermodynamic properties of chemical constituents etc.).

Hypothesis 2: The correlations of selected, well defined properties allow for prediction of thermodynamic properties of apatites (ΔH^o_f, ΔG^o_f, S^o_f, ΔC^o_{pf}) with the precision much better than any other theoretical method of calculation.

To address the objectives and hypothesis of the project, the following research is proposed:

1. Determination and quantification of correlations between existing thermodynamic data and the properties of apatites
2. Calculation of predicted, still unknown values of thermodynamic data;
3. Verification of predicted values by set of dissolution experiments and direct calorimetric measurements.

The structure of apatites, corresponding to the general chemical formula $M_5(AO_4)_3X$, is very flexible and allows for numerous substitutions. The position of a bivalent cation M^{2+} can be filled with Ca^{2+}, Pb^{2+}, Ba^{2+}, Sr^{2+}, Na^{+}, Ce^{3+}, La^{3+}, Y^{3+}, Bi^{3+}, $REE^{3+,2+}$, Th^{4+},$U^{4+,6+}$, etc. At trivalent oxyanion position AO_4^{3-}, A may stand for P^{5+}, As^{5+}, V^{5+}, Si^{4+}, S^{6+}, etc. A monovalent X position is in most cases filled with F, Cl, OH, or O, and can be also fully substituted by Br and I. Partial carbonate CO_3^{2-} substitution for X or for AO_4^{3-} is also often observed. Due to the rich, diverse chemistry of the apatites, there is over 75 minerals which crystallize with apatite structure and a large number of analog synthetic compositions which are recently being studied. Despite the fact that crystallographic properties of many apatites have been described, the thermodynamic properties are much less known. Due to very low solubilities of apatites in general, as well as the tendency of hydroxylapatites for incongruent dissolution, experimental determination of thermodynamic properties is relatively difficult and the literature on this matter is still quite sparse. This, among others, justifies the proposed effort: proposed new method of calculation will allow for estimation (prediction) of many missing data based on current state of knowledge and previously determined, precise experimental data.

Preliminary calculations indicate that useful correlations between existing data for apatites can be found and utilized for this purpose. For verification of calculated values, a synthesis of pure, well defined analogs of natural apatites is planned. Synthetic phases will be used in dissolution experiments. Such experiments are suitable for determination of thermodynamic properties of several, but not for all apatites. Therefore, a complementary method will be used: direct measurement using calorimetry. This method can be used for all apatites but doesn't allow for direct determination of all thermodynamic functions. This way, the approach is complementary and, if proven successful, will be applied to other mineral groups in the future.

The novelty of the project stems from the fact that for the first time strong systematic variations of various properties of minerals (apatites) and their chemical constituents are observed and utilized for correlation, interpolation and extrapolation. Apatite group minerals are particularly suited for the project because there are many apatite species. Several apatites are well characterized providing relatively large set of data for the analysis and calculations. On the other hand, numerous data are still missing and needed and can be determined from existing trends. This way the results of this basic research will have significant impact on the development of this research field. The method is new and carries a potential for being developed in the future and expanded to other groups of minerals.