

Energy levels and crystal-field parameters for Pr^{3+} and Nd^{3+} ions in rare earth (RE) tellurium oxides $\text{RE}_2\text{Te}_4\text{O}_{11}$ revisited-ascent/descent in symmetry method applied for triclinic site symmetry.

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Rok wydania

2011

Czasopismo

Optical Materials

Numer woluminu

33

Strony

1147-1161

DOI

10.1016/j.optmat.2011.01.027

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Triclinic site symmetry presents considerable challenges in the studies of energy levels and crystal-field parameters (CFPs) for rare earth (RE) ions in crystals. Assignment of the spectral features to the irreducible representations of low symmetry point groups is difficult and may be unreliable. Fittings of large number of CFPs, even if the number of the available experimental energy levels is sufficient, often yield multiple solutions with relatively low and close *rms* deviations. These challenges call for better methods of fitting and analysis of CFPs. In this paper, we employ the ascent/descent in symmetry (ADS) method and three computational approaches: (i) a crystallographic data analysis program to identify approximated higher symmetry, (ii) the superposition model (SPM) analysis, and (iii) the pseudosymmetry axes method (PAM) for the combined coordination factors obtained using SPM. As a case study, the experimental CF splittings of Pr^{3+} and Nd^{3+} ions at triclinic C_1 sites in tellurium oxides $\text{RE}_2\text{Te}_4\text{O}_{11}$ are re-analyzed. Two alternative ADS chains $C_1 \leftrightarrow C_2 \leftrightarrow D_2$ and $C_1 \leftrightarrow C_s \leftrightarrow C_{2v}$ were independently obtained. For each approximation of the actual C_1 symmetry of the REO_8 polyhedron in $\text{RE}_2\text{Te}_4\text{O}_{11}$, the ligands' positions are determined and used in SPM to calculate CFP sets, which are used as starting for additional fittings. Comparative analysis of the fitted and calculated CFP sets enables assignment of appropriate axis system to the fitted CFP sets, thus avoiding the ambiguities occurring in previous ADS applications. The very good compatibility and consistency of the newly determined CFP sets indicate high reliability of both approaches. These CFP sets were used to simulate magnetic susceptibility data for polycrystalline samples of $\text{Pr}_2\text{Te}_4\text{O}_{11}$ and $\text{Nd}_2\text{Te}_4\text{O}_{11}$. Wider applications of the proposed procedures in optical spectroscopy studies of low symmetry systems may improve reliability of the CFP sets reported in literature.

Słowa kluczowe

Optical spectroscopy, Crystal (ligand) field parameters, Triclinic site symmetry, $\text{RE}_2\text{Te}_4\text{O}_{11}$, Rare earth tellurium oxides, Pr^{3+} and Nd^{3+} ions

Adres publiczny

<https://doi.org/10.1016/j.optmat.2011.01.027>

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-10-07 09:44:46

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/uzZUt0h>.