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M.G. Brik, C.N. Avram, N.M. Avram. Comparative study of crystal field effects for Ni ion in LiGaO, MgF and AgCl crystals. *Journal of Physics and Chemistry of Solids*, 2009, 69 (7), pp.1796. 10.1016/j.jpcs.2008.01.004 . hal-00526542

HAL Id: hal-00526542

<https://hal.science/hal-00526542>

Submitted on 15 Oct 2010

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Author's Accepted Manuscript

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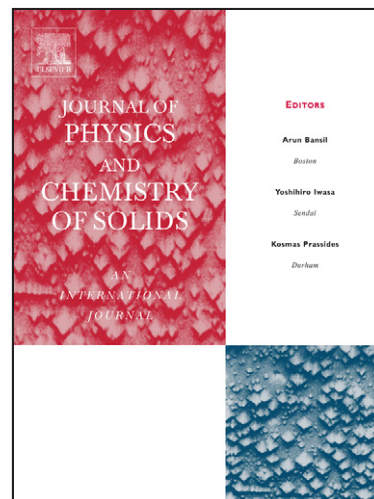
PII: S0022-3697(08)00008-5
DOI: doi:10.1016/j.jpcs.2008.01.004
Reference: PCS 5356

To appear in: *Journal of Physics and Chemistry of Solids*

Received date: 17 May 2007
Revised date: 2 July 2007
Accepted date: 1 January 2008

Cite this article as: M.G. Brik, C.N. Avram and N.M. Avram, Comparative study of crystal field effects for Ni²⁺ ion in LiGa₅O₈, MgF₂ and AgCl crystals, *Journal of Physics and Chemistry of Solids* (2008), doi:10.1016/j.jpcs.2008.01.004

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Comparative study of crystal field effects for Ni²⁺ ion in LiGa₅O₈, MgF₂ and AgCl crystals**M.G. Brik¹, C.N. Avram², N.M. Avram²**

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Abstract

Exchange charge model of crystal field was used to calculate the crystal field parameters and model the energy levels for Ni²⁺ ion in LiGa₅O₈, MgF₂, and AgCl crystals. Calculated energy levels (including splitting of the orbital triplets) are in good agreement with experimental absorption spectra. Covalent effects were shown to play an important role in all considered crystals. Bilinear forms built up from the overlap integrals between (Ni²⁺-Cl⁻) → (Ni²⁺-O²⁻) → (Ni²⁺-F⁻) pairs were considered as a quantitative measure of the covalent (nephelauxetic) effects.

1. Introduction

Crystals doped with Ni²⁺ ion are characterized by broad absorption bands in visible and infrared spectral regions [1]. After doping, Ni²⁺ ions may occupy both octahedral and tetrahedral sites [1-3]. Numerous studies of various aspects related to the Ni²⁺-doped crystals can be found in the literature [4-24; this list of references is rather representative]. In this paper we present the results of application of the exchange charge model of crystal field [25] to the calculation of the CFPs values and energy levels for Ni²⁺ in three crystals: LiGa₅O₈, MgF₂, and AgCl. In these hosts Ni²⁺ ion occupies octahedral positions, and we would follow how the variation of ligands affects the properties of impurity ion. Calculated results are compared with experimental absorption spectra available in the literature; covalent effects for all considered hosts are compared and discussed.

The paper is organized as follows: in the next section a short review of crystallographic data for three considered crystals is given. Then we proceed with a brief description of the

calculating technique and discussion of the obtained results. Finally, the paper is concluded with a short summary.

2. Crystal structures of LiGa_5O_8 , MgF_2 , and AgCl

LiGa_5O_8 crystallizes in an inverse spinel structure [26], space group $P4332$, lattice constants is 8.203 \AA , 4 formula units in one unit cell [27]. Fig. 1 shows one unit cell of LiGa_5O_8 . After doping Ni^{2+} substitutes for Ga^{3+} ions (it should be noted here that there are two inequivalent gallium positions: octahedral, and tetrahedral, with Ga–O distance 1.776 \AA [27]). According to Ref. [26], Ni^{2+} exhibits preference to occupy octahedral site.

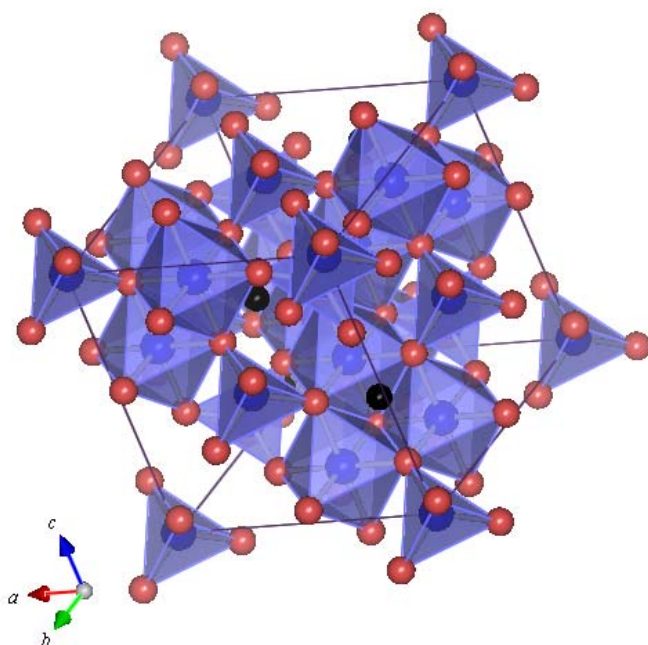


Fig. 1. One unit cell of LiGa_5O_8 . Two kinds of coordination polyhedra formed by oxygen ions around gallium ions are shown. Lithium ions are shown by black spheres. Drawn with VENUS developed by Izumi and Dilanian.

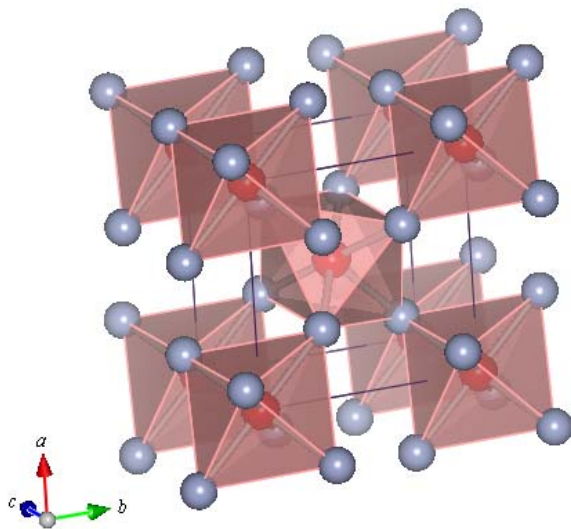


Fig. 2. One unit cell of MgF_2 . Drawn with VENUS developed by Izumi and Dilanian

MgF_2 , according to Ref. [28], has a rutile-type structure, with space-group $P42/mnm$, two formula units in a unit cell and lattice constants $a = 4.6213 \text{ \AA}$, $c = 3.0159 \text{ \AA}$. There is only one Mg^{2+} position (available for Ni^{2+}) at the center of F^- octahedron with Mg-F bonds 1.979 \AA (two bonds) and 1.984 \AA (four bonds) [28], with the last circumstance suggesting a slight deformation of the MgF_6 octahedron. Fig. 2 shows one unit cell of MgF_2 .

Finally, the structure of AgCl is the simplest one among the considered crystals. It crystallizes in a cubic structure with space group $Fm3m$, four formula units in one unit cell and lattice constant 5.5463 \AA [29].

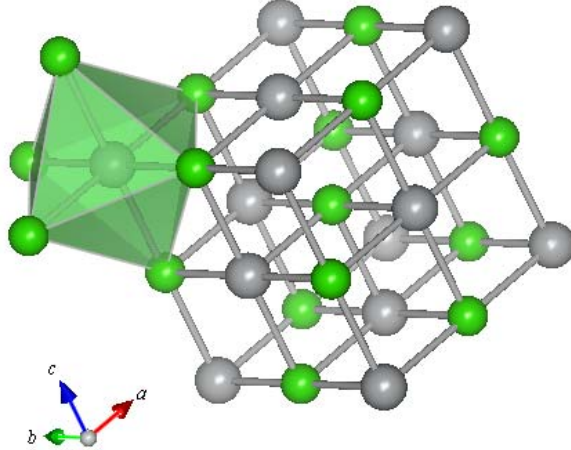


Fig. 3. One unit cell of AgCl. For the sake of simplicity, only one coordination polyhedron formed by chlorine ions around silver ions is shown. Lithium ions are shown by black spheres. Drawn with VENUS developed by Izumi and Dilanian

Ag^+ ions (substituted for by Ni^{2+} ions) are at the centers of the chlorine octahedra with Ag–Cl distance 2.773 Å [29]. Structural data from Refs. [27–29] were used to calculate the crystal field parameters (CFPs) acting on Ni^{2+} ions.

3. Exchange charge model (ECM) of crystal field

One of possible ways of representing the energy levels of $3d$ ions in a crystal field is to use the following crystal field Hamiltonian [25]:

$$H = \sum_{p=2,4} \sum_{k=-p}^p B_p^k O_p^k, \quad (1)$$

where O_p^k are the linear combinations of spherical operators (which act on the angular parts of a $3d$ ion wave functions), and B_p^k are CFPs containing all information about geometrical structure of an impurity center. Salient feature of the ECM is that these parameters can be written as a sum of two terms [25]:

$$B_p^k = B_{p,q}^k + B_{p,s}^k. \quad (2)$$

The first contribution arises from the electrostatic interaction between a $3d$ ion and ions of crystal lattice (treated as point charges, without taking into account their electron structure), and the second one is proportional to the overlap of the wave functions of a central ion and ligands. This term accounts for all effects of the covalent bond formation and exchange interaction, and inclusion of these effects significantly improves agreement between the calculated and experimentally observed energy levels. Expressions for calculating both contributions to the CFPs in the case of $3d$ -ion are as follows [25]:

$$B_{p,q}^k = -K_p^k e^2 \langle r^p \rangle \sum_i q_i \frac{V_p^k(\theta(i), \varphi(i))}{R(i)^{p+1}}, \quad (3)$$

$$B_{p,s}^k = K_p^k e^2 \frac{2(2p+1)}{5} \sum_i \left(G_s S(s)_i^2 + G_\sigma S(\sigma)_i^2 + \gamma_p G_\pi S(\pi)_i^2 \right) \frac{V_p^k(\theta_i, \varphi_i)}{R_i}. \quad (4)$$

The sums are carried out over lattice ions denoted by i with charges q_i ; $R(i), \theta(i), \varphi(i)$ are the spherical coordinates of the i -th ion of crystal lattice in the system of reference centered at the central ion. The averaged values $\langle r^p \rangle$ of p -th power of the central ion electron radial coordinate are given in Ref. [30]. The values of the numerical factors K_p^k, γ_p and expressions for the polynomials V_p^k are given in [25]. $S(s), S(\sigma), S(\pi)$ correspond to the overlap integrals between d -functions of the central ion and p - and s -functions of the ligands: $S(s) = \langle d0 | s0 \rangle, S(\sigma) = \langle d0 | p0 \rangle, S(\pi) = \langle d1 | p1 \rangle$. G_s, G_σ, G_π are dimensionless adjustable parameters of the model, whose values can be determined from the positions of the first three absorption bands. We assume that they can be approximated to a single value, i.e. $G_s = G_\sigma = G_\pi = G$, that can be estimated from only one (the lowest in energy) absorption band. This is usually a reasonable approximation. The strong advantage of the ECM is that if the G parameter is determined to fit the first absorption band, the other energy levels, located higher in energy, will also fit experimental spectra fairly well.

Numerous applications of the ECM to the analysis of rare-earth and transition metal doped crystals [25, 31–36 and references therein] show this model to be a powerful and reliable tool for analysis and interpretation of crystal field effects and optical absorption spectra.

4. Results of calculations and discussion

The CFPs were calculated using the ionic positions obtained from structural data [27–29]. To ensure convergence of CFPs (especially those ones of the second rank), large clusters were

considered. For example, in the cases of LiGa_5O_8 and MgF_2 56630 and 50061 ions were taken into account, respectively. In the case of AgCl only 9253 ions were involved into lattice summations (but this number was more than sufficient for fast convergence of the CFPs, since in this case there are no second rank parameters). The overlap integrals between Ni^{2+} and O^{2-} , F^- , Cl^- ions were calculated numerically using the wave functions from Refs. [37, 38]; for convenience, the obtained results were approximated by exponential functions shown in Table 1.

Table 1

Overlap integrals between Ni^{2+} and O^{2-} , F^- , and Cl^- ions (r is measured in atomic units)

	$\text{Ni}^{2+} - \text{O}^{2-}$	$\text{Ni}^{2+} - \text{F}^-$	$\text{Ni}^{2+} - \text{Cl}^-$
$S_s = \langle d0 s0 \rangle$	$-0.99799 \exp(-0.73145r)$	$2.37820 \exp(-1.01880r)$	$-1.82070 \exp(-0.85599r)$
$S_\sigma = \langle d0 p0 \rangle$	$0.84696 \exp(-0.68325r)$	$1.07440 \exp(-0.72669r)$	$0.81606 \exp(-0.59570r)$
$S_\pi = \langle d1 p1 \rangle$	$1.13280 \exp(-0.86486r)$	$1.58920 \exp(-0.98151r)$	$1.54200 \exp(-0.85907r)$

The calculated CFPs values are shown in Table 2 (point charge and exchange charge contributions are denoted by PCC and ECC, respectively, and shown separately). As seen from the Table, the ECC value is always greater than its PCC counterpart. Values of the ECM parameter G were determined from the positions of the first absorption band in the corresponding absorption spectra and are also shown in the last line of Table 2.

Obtained values of CFPs were used to diagonalize the crystal field Hamiltonian (1) in the space spanned by all 25 wave functions of 5 LS terms of Ni^{2+} (^3P , ^3F , ^1S , ^1D , ^1G). Spin-orbit interaction was not considered, since the absorption bands in the experimental spectra are broad and no fine structure is observed. Calculated energy levels are shown in Table 3.

As seen from this Table, the calculated values are in good agreement with experimental data. It also should be pointed out that the calculation of energy levels for $\text{Ni}^{2+}:\text{LiGa}_5\text{O}_8$ in Ref. [26] were performed in a cubic approximation, i.e. neglecting the low-symmetry component of crystal field, which was completely accounted for in our calculations. Figures 4–6 illustrate how the calculated energy levels (including splitting of the orbital triplets in LiGa_5O_8 and MgF_2) are related to the experimental absorption spectra. The width of the absorption bands corresponding to the transitions to the spin-triplet states is well reproduced by our calculations; positions of the absorption lines of small intensities, which correspond to the transitions to the spin-singlet states, also match well the calculated energy levels.

Table 2. CFPs values (in cm^{-1}) for Ni^{2+} ions in LiGa_5O_8 , MgF_2 , and AgCl crystals

	LiGa_5O_8			MgF_2			AgCl		
	PCC	ECC	Total value	PCC	ECC	Total value	PCC	ECC	Total value
B_2^{-2}	980.4	–	980.4	788.4	942.4	1730.8	–	–	–
B_2^{-1}	-6503.2	–	-6503.2	–	–	–	–	–	–
B_2^0	-387.6	–	-387.6	-95.4	829.8	734.4	–	–	–
B_2^1	1961.0	–	1961.0	–	–	–	–	–	–
B_2^2	1163.2	–	1163.2	–	–	–	–	–	–
B_4^{-4}	0.0	–	0.0	–	–	–	–	–	–
B_4^{-3}	421.5	–	421.5	–	–	–	–	–	–
B_4^{-2}	-50.8	–	-50.8	-1910.6	-8182.7	-10093.3	–	–	–
B_4^{-1}	-60.2	–	-60.2	–	–	–	–	–	–
B_4^0	656.6	1912.0	2568.6	-100.4	-258.4	-358.8	74.5	1679.0	1753.5
B_4^1	25.4	–	25.4	–	–	–	–	–	–
B_4^2	94.0	–	94.0	–	–	–	–	–	–
B_4^3	178.0	–	178.0	–	–	–	–	–	–
B_4^4	3189.2	9559.8	12749.0	-1117.7	-5467.8	-6585.5	372.5	8394.9	8767.4
G		4.35			1.87			19.23	

Table 3

Observed and calculated (this work) energy levels (in cm^{-1}) of Ni^{2+} ion in LiGa_5O_8 , MgF_2 and AgCl^1

Energy levels (O_h group notations)	LiGa ₅ O ₈				MgF ₂		AgCl	
	This work		Ref. [26]		Calculated, this work	Observed, [1, 39]	Calculated, this work	Observed, [40]
	Calculated	Ave- raged	Observed	Calcu- lated				
³ A _{2g} (³ F)	0 9275	0	0	0	0 7307	0	0	0
³ T _{2g} (³ F)	9949 10089	9771	9770	9770	7346 7751	7500	6680	6680
¹ E _g (¹ D)	12957 13014	12986	12987	13030	15573 15595	15600	12206	12470
³ T _{1g} (³ F)	15455 16044 16384 21437	15961	16050	15940	11906 12672 13113 22177	11900 12500 13300	11222	11250
¹ T _{2g} (¹ D)	22119 22786	22114	22300	22450	22314 22935	–	18489	18480
¹ A _{1g} (¹ G)	22865 24829	22865	–	–	24858 23548	– 23500	19779	–
³ T _{1g} (³ P)	27096 28332 26015	26752	26740	26780	24840 25472 27215	24800 25300	20923	20920
¹ T _{1g} (¹ G)	26714 27807	26845	–	–	27527 28362	–	22646	–
¹ E _g (¹ G)	33219 33582	33401	–	–	32521 32637	–	27437	–
¹ T _{2g} (¹ G)	34527 36057 36272	35619	–	–	33146 33846 34062	–	27834	–
¹ A _{1g} (¹ S)	56770	56770	–	–	61649	–	49288	–
Racah parameters <i>B, C</i>	881, 3225				995, 4192		807, 3141	

¹ Note that the order of the ¹E_g (¹D) and ³T_{1g} (³F) levels in MgF₂ and AgCl are inverted with that for LiGa₅O₈.

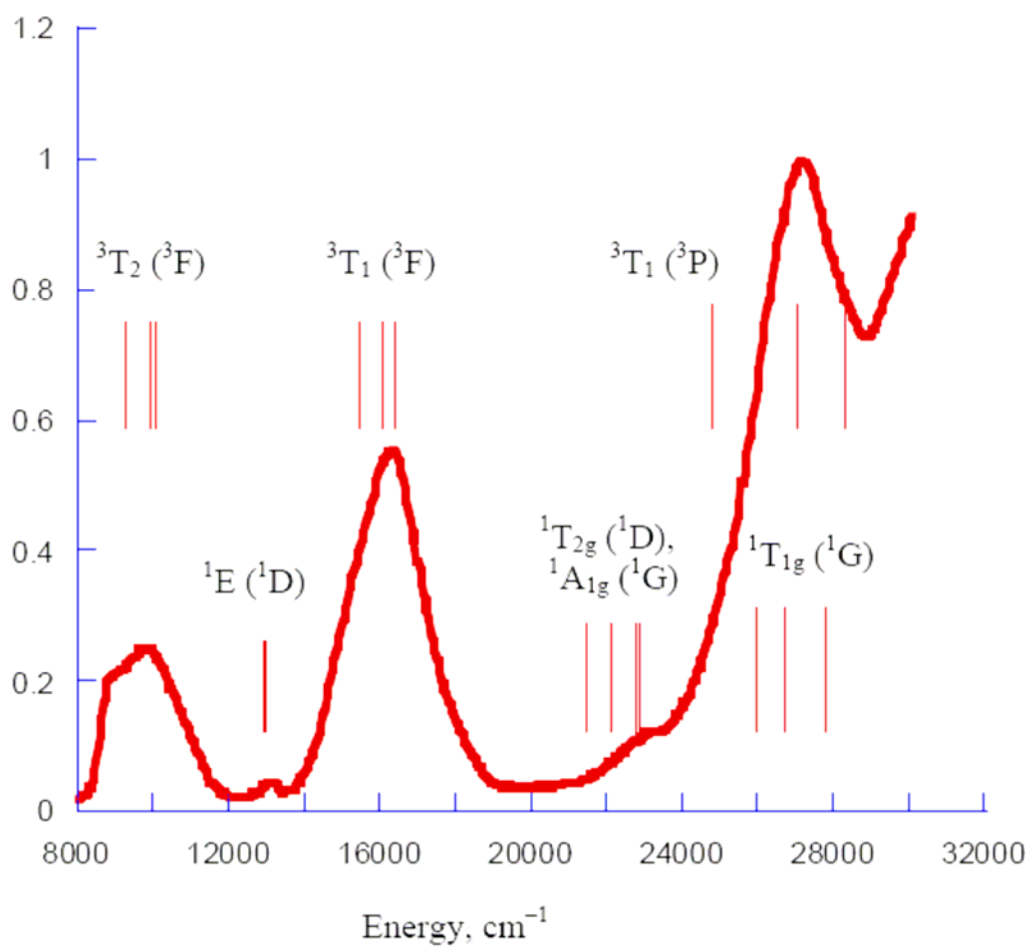


Fig. 4. Absorption spectra [26] of $\text{LiGa}_5\text{O}_8:\text{Ni}^{2+}$. Calculated in this work Ni^{2+} energy levels are shown by vertical lines.

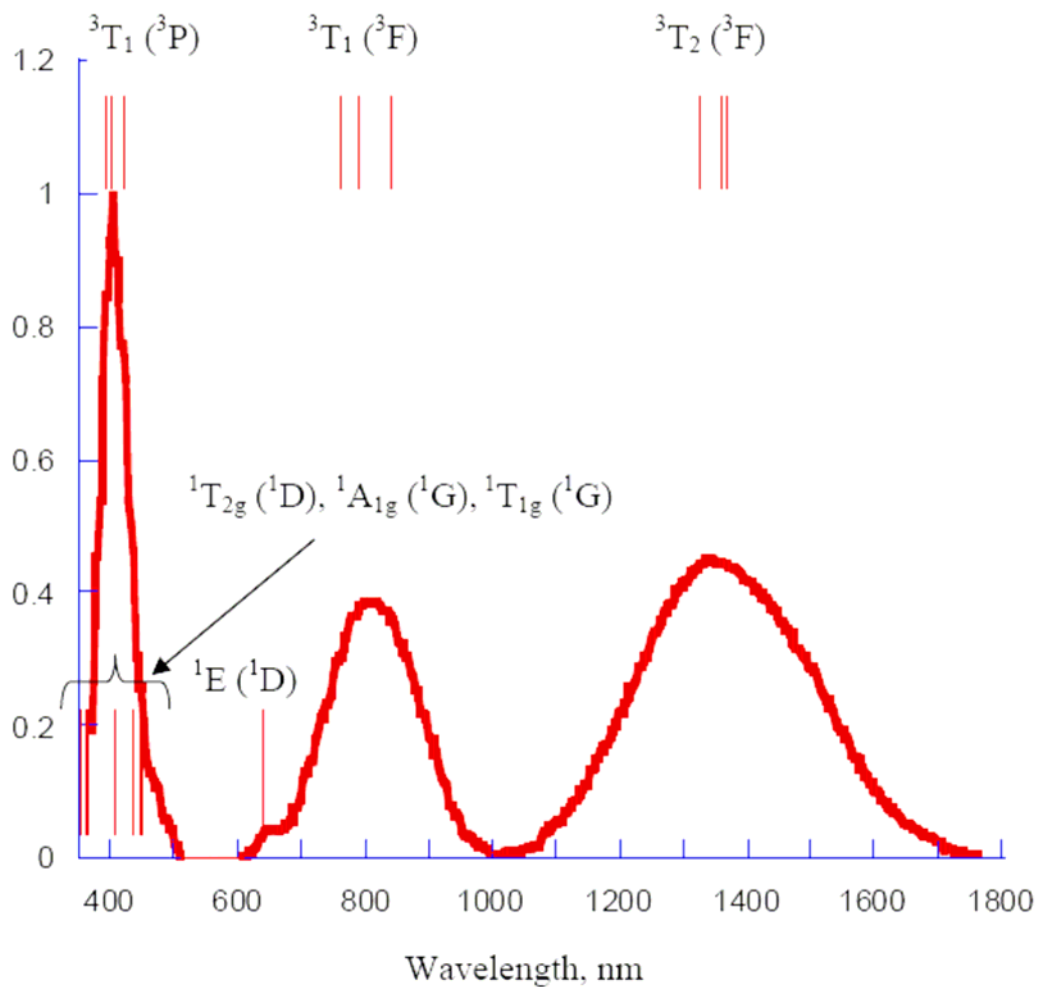


Fig. 5. Absorption spectra [1] of MgF₂:Ni²⁺. Calculated in this work Ni²⁺ energy levels are shown by vertical lines.

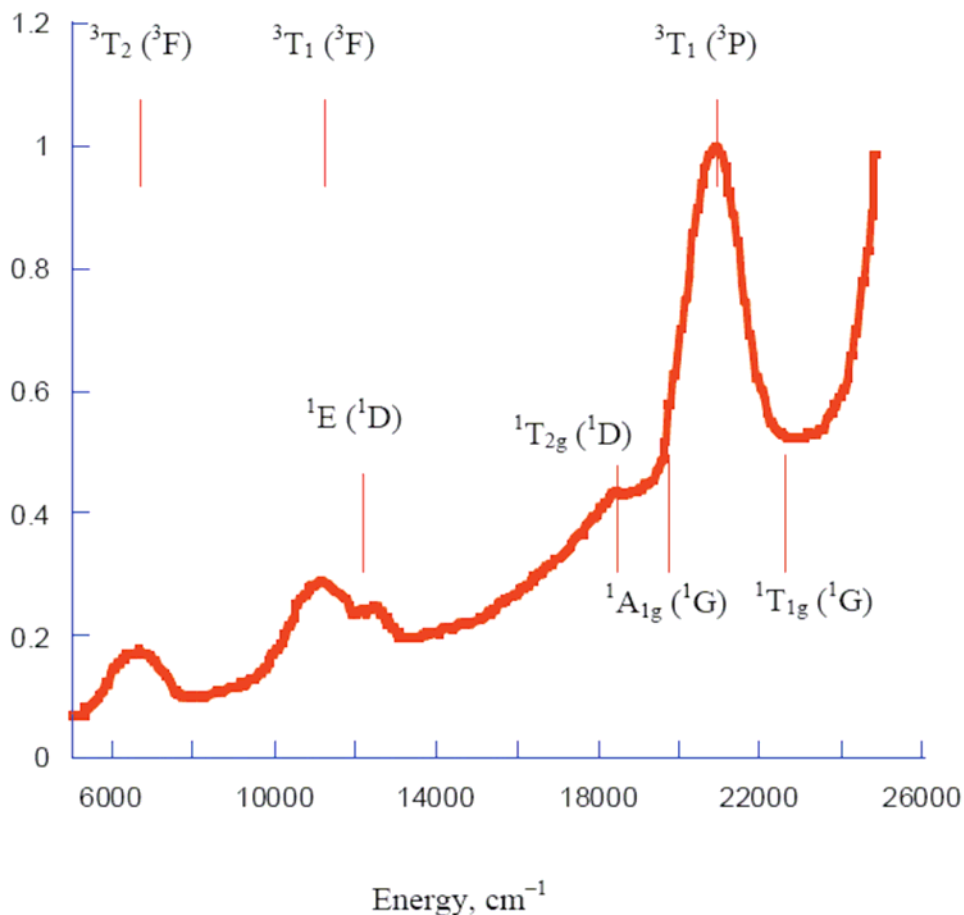


Fig. 6. Absorption spectra [40] of AgCl:Ni²⁺. Calculated in this work Ni²⁺ energy levels are shown by vertical lines.

Comparison of the Racah parameters for Ni²⁺ in crystals (Table 3) with values for free Ni²⁺ ion ($B = 1068 \text{ cm}^{-1}$, $C = 4457 \text{ cm}^{-1}$ [41]) shows that there is significant reduction of these parameters due to covalency. This reduction is the greatest in AgCl crystal, the smallest in MgF₂ and medium in LiGa₅O₈. In other words, the Ni–Cl bonds are the most covalent, and the Ni–F bond are most ionic. This conclusion is supported by Figures 7 and 8, which show the bilinear forms $S_2 = G(S(s)_i^2 + S(\sigma)_i^2 + S(\pi)_i^2)$ and $S_4 = G(S(s)_i^2 + S(\sigma)_i^2 + \gamma_4 S(\pi)_i^2)$ constructed from overlap integrals from Table 1.

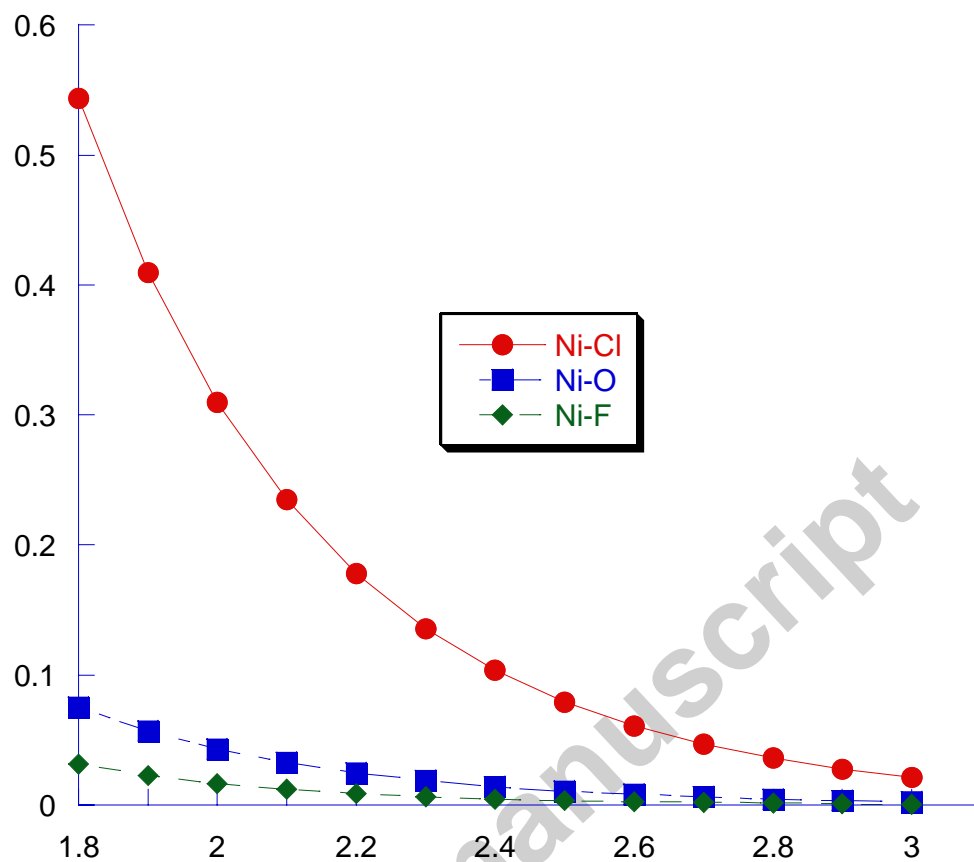


Fig. 7. Dependence of the $S_2 = G(S(s)_i^2 + S(\sigma)_i^2 + S(\pi)_i^2)$ bilinear form on distance for $\text{Ni}^{2+}-\text{Cl}^-$, $\text{Ni}^{2+}-\text{O}^{2-}$, $\text{Ni}^{2+}-\text{F}^-$ ions.

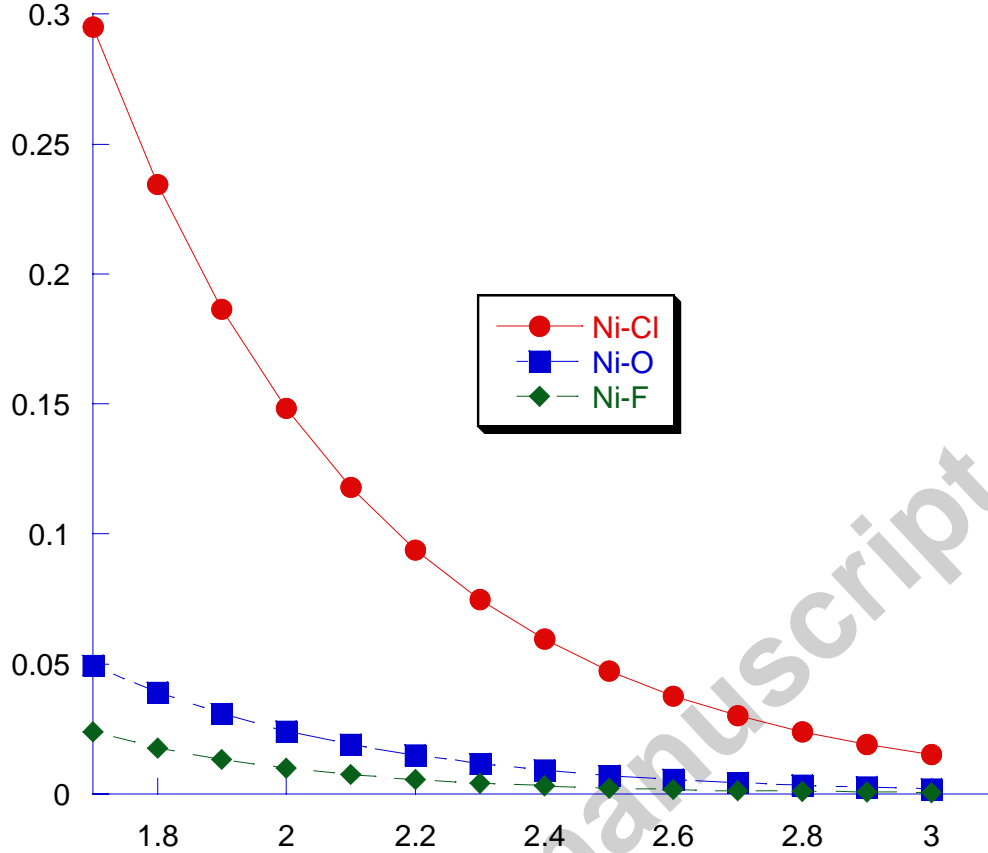


Fig. 8. Dependence of the $S_4 = G(S(s)_i^2 + S(\sigma)_i^2 + \gamma_4 S(\pi)_i^2)$ bilinear form on distance for $\text{Ni}^{2+}-\text{Cl}^-$, $\text{Ni}^{2+}-\text{O}^{2-}$, $\text{Ni}^{2+}-\text{F}^-$ ions.

Decreasing values of S_2 and S_4 in the $(\text{Ni}^{2+}-\text{Cl}^-) \rightarrow (\text{Ni}^{2+}-\text{O}^{2-}) \rightarrow (\text{Ni}^{2+}-\text{F}^-)$ sequence follow decreasing degree of covalent bonds and increasing values of the Racah parameters B , C in the $\text{AgCl}:\text{Ni}^{2+} \rightarrow \text{LiGa}_5\text{O}_8:\text{Ni}^{2+} \rightarrow \text{MgF}_2:\text{Ni}^{2+}$ series. These results which emphasized the specific role of the Ni ions doped in the title crystals could be added to that of paper [42] which has been observed during investigations of the spectra for Ni doped highly anisotropic crystals.

5. Conclusions

Consistent calculations of the CFPs values and energy levels for Ni^{2+} ions in three crystals LiGa_5O_8 , AgCl , and MgF_2 were performed in the present paper using the exchange charge model of crystal field. For the first time for the considered crystals the CFPs values were calculated from crystal structure data, with taking into account low symmetry component of crystal field.

Calculated energy levels (including splitting of the orbital triplets) match well available in the literature absorption spectra. A special attention was paid to analysis of the covalent effects, which were represented quantitatively by the bilinear forms constructed from the overlap integrals between Ni^{2+} and ligands' wave functions. Enhancement of the covalent (nephealuxetic) effects was shown to be connected with greater values of the overlap integrals.

Calculated complete energy level schemes can be used for analysis of the Ni^{2+} excited state absorption in the considered hosts, and the sets of CFPs can be used as initial (starting) sets for analysis of Ni^{2+} energy levels in other isostructural crystals.

Accepted manuscript

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