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Investigations of the spin-Hamiltonian parameters and tetragonal distortions due to Jahn–Teller effect for the monovalent d^9 (Ni^+, Pd^+, Pt^+) impurity centers in AgCl crystals

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ABSTRACT

When the monovalent md^9 ions Ni^+ ($3d^9$), Pd^+ ($4d^9$) and Pt^+($5d^9$) substitute for the Ag^+ ions in AgCl crystal, the cubic chlorine octahedron surrounding Ag^+ in the host AgCl crystal distorts into the tetragonally elongated octahedron in the md^9 impurity center owing to the Jahn–Teller effect. The spin-Hamiltonian parameters (g factors $g_{||}$, $g_\perp$ and hyperfine structure constants $A_{||}$, $A_\perp$) of the tetragonal md^9 centers in AgCl are calculated from the high-order perturbation formulas based on the cluster approach, in which the admixture between d orbitals of d^n ion and p orbitals of ligand ion via covalence effect are taken into account. From the calculations, the spin-Hamiltonian parameters of these tetragonal md^9 centers in AgCl are explained reasonably and the tetragonal distortions (characterized by the tetragonal elongation $\Delta R = R_{||} - R_\perp$, where $R_{||}$ and $R_\perp$ denote the metal–ligand distances parallel with and perpendicular to the tetragonal axis) of these centers due to Jahn–Teller effect are obtained. The results are discussed.

1. Introduction

d^9 ions are the well-known Jahn–Teller ions because when they occupy a regular (or cubic) octahedral site, the ground orbital state is doublet ^2E. This degenerate ground state is unstable, so a Jahn–Teller distortion may occur to remove the degeneracy. The doublet ^2E in tetragonal crystal field can be split into either singlet $^2B_1(|d_{x^2-y^2}\rangle)$ or $^2A_1(|d_{z^2}\rangle)$, corresponding to elongated or compressed tetragonal field, so a d^9 ion in a cubic octahedron will undergo a Jahn–Teller distortion from cubic to tetragonal. Generally speaking, the elongated distortion is by far the most common [1–4]. For example, for the monovalent d^9 ion series Ni^+ ($3d^9$), Pd^+ ($4d^9$) and Pt^+ ($5d^9$) in cubic AgCl crystal, the tetragonal d^9 impurity centers were found and their anisotropic spin-Hamiltonian parameters (g factors $g_{||}$, $g_\perp$ and hyperfine structure constants $A_{||}$, $A_\perp$) were reported from electron paramagnetic resonance (EPR) experiments [5,6]. The md^9 ($m = 3, 4, 5$) ions at Ag^+ site of AgCl are isovalent substitution, where no charge compensator is required. So the tetragonal distortion of d^9 ion centers in AgCl should be due to Jahn–Teller effect rather than charge compensation. So far, no theoretical studies for the spin-Hamiltonian parameters of md^9 ion series in AgCl have been performed. Considering that (i) although many studies for the spin-Hamiltonian parameters of $3d^n$ ions in crystal were made, such studies for $4d^n$ and $5d^n$ ions in crystals are scarce; (ii) AgCl is an interesting material used in the fields of photography, ionic conduction, laser and sensors [7–11] and (iii) the spin-Hamiltonian parameters of a paramagnetic ion in crystals are sensitive to its immediate environment, so the studies of spin-Hamiltonian parameters can acquire information on the tetragonal distortion (characterized by $\Delta R = R_{||} - R_\perp$, where $R_{||}$ and $R_\perp$ denote the metal–ligand distances parallel with and perpendicular to the tetragonal axis) of md^9 clusters in AgCl crystal, the theoretical studies of the spin-Hamiltonian parameters for md^9 ion series in AgCl are of significance. In this paper, we calculate the spin-Hamiltonian parameters and study the tetragonal distortion due to Jahn–Teller effect for md^9 ions in AgCl by using the high-order perturbation formulas based on the cluster approach. The results are discussed.

2. Calculation

According to the cluster approach for a d^n octahedral cluster, the one-electron basis functions can be expressed as the linear com-

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Table 1
The group overlap integrals $S_{\mathrm{dp}}(\gamma)$, the crystal field parameters Dq, the molecular orbital coefficients λ_γ and N_γ, the tetragonal elongations ΔR and core polarization constants κ for $m\mathrm{d}^9$ ions Ni⁺, Pd⁺ and Pt⁺ in AgCl crystals.

	S_{dp} (e_g)	S_{dp} (t_2)	Dq (cm^{-1})	λ_γ	N_t	N_e	ΔR (Å)	κ
AgCl:Ni⁺	0.01163	0.00296	560	0.1977	0.9805	0.9788	0.09	
AgCl:Pd⁺	0.03885	0.01065	800	0.5019	0.8900	0.8801	0.08	0.5476
AgCl:Pt⁺	0.05400	0.01506	1500	0.5756	0.8611	0.8471	0.06	1.5437

Table 2
The spin–orbit parameters (in cm^{-1}), the orbital reduction factors and the dipolar hyperfine constants (in 10^{-4} cm^{-1}) for $m\mathrm{d}^9$ ions Ni⁺, Pd⁺ and Pt⁺ in AgCl crystals.

Crystals	ζ	ζ'	k	k'	P	P'
AgCl:Ni⁺	592.6	569.6	0.9812	0.9437		
AgCl:Pd⁺	1183.2	1054.4	0.9002	0.7041	−42.8382	−43.3158
AgCl:Pt⁺	3216.0	3022.0	0.8772	0.6376	312.8846	318.0427

bination of d orbitals $|d_\gamma\rangle$ of d^n ion and p orbitals $|p_\gamma\rangle$ of ligand [12–14],

$$|\psi_\gamma\rangle = N_\gamma^{1/2}(|d_\gamma\rangle - \lambda_\gamma|p_\gamma\rangle) \tag{1}$$

in which γ (=t_2 or e_g) denotes the irreducible representation of O_h group. N_γ and λ_γ are the normalization coefficient and the orbital mixing coefficient.

From the basis functions, we have two spin–orbit parameters ζ, ζ', two orbital reduction factors k, k' and two dipolar hyperfine structure constants P, P' (where ζ, k and P are related to the interaction within t_2 states and the others to that between t_2 and e_g states), i.e. [12–14],

$$\begin{aligned}
&\zeta = N_t^2\left(\zeta_\mathrm{d}^0 + \frac{\lambda_t^2\zeta_\mathrm{p}^0}{2}\right), && \zeta' = (N_tN_\mathrm{e})\left(\zeta_\mathrm{d}^0 - \frac{\lambda_t\lambda_\mathrm{e}\zeta_\mathrm{p}^0}{2}\right)\\
&k = N_t^2\left[1 + 2\lambda_tS_{\mathrm{dp}}(t_{2g}) + \frac{\lambda_t^2}{2}\right], && k' = (N_tN_\mathrm{e})\left[1 + \lambda_tS_{\mathrm{dp}}(t_{2g}) + \lambda_\mathrm{e}S_{\mathrm{dp}}(e_g) - \frac{\lambda_t\lambda_\mathrm{e}}{2}\right]\\
&P = N_t^2P_0, && P' = N_tN_\mathrm{e}P_0
\end{aligned} \tag{2}$$

where ζ_d^0 and ζ_p^0 are the spin–orbit parameters of free d^n ion and free ligand ion. P_0 is the corresponding constant of free d^n ion. $S_{\mathrm{dp}}(\gamma)$ are the group overlap integrals of $|d_\gamma\rangle$ and $|p_\gamma\rangle$ orbitals. For $m\mathrm{d}^9$ ion in AgCl under study, we have ζ_p^0 (Cl⁻) ≈ 587 cm^{-1} [15], ζ_d^0 (Ni⁺) ≈ 605 cm^{-1} [16], ζ_d^0 (Pd⁺) ≈ 1420 cm^{-1} and ζ_d^0 (Pt⁺) ≈ 4240 cm^{-1}. The values of ζ_d^0 (Pd⁺) and ζ_d^0 (Pt⁺) are estimated by a extrapolation of the values ζ_d^0 (Pd^{n+}) (n = 4, 3, 2) and ζ_d^0 (Pt^{n+}) given in Ref. [17]. The estimated value of ζ_d^0 (Pd⁺) is consistent with that given in Ref. [18], so these values may be suitable. The dipolar hyperfine structure constant P_0 can be calculated from the formula [19] $P = g_\mathrm{e}g_\mathrm{N}\beta\beta_\mathrm{N}\langle r^{-3}\rangle$, where $g_\mathrm{N} = \mu_\mathrm{I}/I$. The expectation value $\langle r^{-3}\rangle \approx 7.20738$ a.u. and 11.29086 a.u. for Pd⁺ and Pt⁺, respectively [20], and I = 5/2 and 1/2, $\mu_\mathrm{I} = -0.6015$ and 0.606 for ^{105}Pd and ^{195}Pt, respectively [21], thus we have

$$P_0(^{105}\mathrm{Pd}^+) \approx -55.3\times10^{-4}\,\mathrm{cm}^{-1}, \quad P_0(^{195}\mathrm{Pt}^+) \approx 436\times10^{-4}\,\mathrm{cm}^{-1} \tag{3}$$

The integrals $S_{\mathrm{dp}}(\gamma)$ can be calculated from the Slater-type self-consistent field (SCF) functions [22,23] and the metal–ligand distance R. The calculated integrals $S_{\mathrm{dp}}(\gamma)$ for $m\mathrm{d}^9$ ion in AgCl (with the metal–ligand distance R ≈ 2.773 Å [24] of AgCl) are listed in Table 1.

Since the observed $g_{||} > g_\perp$, the $m\mathrm{d}^9$ octahedral clusters in AgCl are tetragonally elongated and their ground orbital state is $^2\mathrm{B}_1(|d_{x^2-y^2}\rangle)$. Using the perturbation method similar to that in Ref. [25], the high-order perturbation formulas based on the cluster approach for the spin-Hamiltonian parameters of d^9 ions in a tetragonally elongated octahedron are derived as

$$\begin{aligned}
g_{||} &= g_\mathrm{s} + \frac{8k'\zeta'}{E_1} - \frac{4k\zeta\zeta'}{E_1E_2} - \frac{(k' + g_\mathrm{s}/2)\zeta'^2}{E_2^2}\\
g_\perp &= g_\mathrm{s} + \frac{2k'\zeta'}{E_2} + \frac{2k\zeta'^2 - 2k'\zeta\zeta'}{E_1E_2} - \frac{g_\mathrm{s}\zeta'^2 - k'\zeta\zeta'}{E_2^2} - \frac{2g_\mathrm{s}\zeta'^2}{E_1^2}\\
A_{||} &= P\left(-\kappa - \frac{4}{7}\right) + P'\left[(g_{||} - g_\mathrm{s}) + \frac{3}{7}(g_\perp - g_\mathrm{s})\right]\\
A_\perp &= P\left(\frac{2}{7} - \kappa\right) + \frac{11}{14}P'(g_\perp - g_\mathrm{s})
\end{aligned} \tag{4}$$

where g_s ≈ 2.0023, the value of free d^n ion, κ is the core polarization constant which is sensitive to the even small deformation of the metal electron orbitals and is often taken as an adjustable parameter [26–28]. E_1 and E_2 are the crystal field energy levels and read

$$E_1 = 10Dq, \quad E_2 = 10Dq + 3Ds - 5Dt \tag{5}$$

in which Dq, Ds and Dt are the crystal field parameters. Considering that the superposition model [29,30] enables correlation of crystal

Table 3
The spin-Hamiltonian parameters (g factors and hyperfine structure constant A, A-values are in 10^{-4} cm^{-1}) for the tetragonal $m\mathrm{d}^9$ ion Ni⁺, Pd⁺ and Pt⁺ centers in AgCl crystals.

	$g_{||}$ [a]	$g_\perp$ [a]	$A_{||}$ [a]	$A_\perp$ [a]	g_{iso} [b]	A_{iso} [b]
AgCl:Ni⁺						
Calc.	2.714	2.138			2.330	
Expt. [5]	2.714 (9)	2.138			2.330	
AgCl:Pd⁺						
Calc.	2.648	2.114	17.9	7.4	2.292	10.9
Expt. [6]	2.648 (6)	2.120 (6)	16	8	2.296 (6)	10.7
AgCl:Pt⁺						
Calc.	2.815	2.097	−390.4	−369.9	2.336	−376.7
Expt. [5]	2.815 (4)	2.1 (1)	390.4 [c]		2.338	

[a] The values at low temperature due to the static Jahn–Teller effect.
[b] The values at high temperature due to the dynamic Jahn–Teller effect.
[c] The value given in Ref. [5] is actually the absolute one.

field parameters and the structural data of paramagnetic center in crystals, the tetragonal field parameters Ds and Dt are calculated by using the model, i.e.,

$$Ds = \frac{4}{7}\overline{A_2}(R_0)\left[\left(\frac{R_0}{R_\perp}\right)^{t_2} - \left(\frac{R_0}{R_{||}}\right)^{t_2}\right],$$
$$Dt = \frac{16}{21}\overline{A_4}(R_0)\left[\left(\frac{R_0}{R_\perp}\right)^{t_4} - \left(\frac{R_0}{R_{||}}\right)^{t_4}\right] \quad (6)$$

in which t_k (k = 2, 4) are the power-law exponents, we take $t_2 = 3$ and $t_4 = 5$ [31–35] here. $\overline{A_k}(R_0)$ are the intrinsic parameters with the reference distance R_0. For d^n ions in octahedral clusters, $\bar{A}_4(R_0) = (3/4)Dq$ [29,31,32], where the cubic field parameter Dq is estimated from the optical spectra of the studied system. For md^9 ions in AgCl, no optical spectral data were reported. We estimate the parameters Dq from the following points: (i) for the AX_6 octahedra with the same metal ion A and ligand X, the value of Dq increases with the increase in the valent state of ion A, and (ii) for the isovalent md^n ion series, the parameter Dq increases with the increasing value of m [36]. The estimated values of Dq for md^9 ions in AgCl from many optical spectral data summarized in Ref. [36] are given in Table 1. The ratio $\overline{A_2}(R_0)/\overline{A_4}(R_0) \approx 10 \pm 2$, 6 ± 2 and 5 ± 2 for 3d^n, 4d^n and 5d^n ions in crystals, respectively [31–35,37]. We take $\overline{A_2}(R_0)/\overline{A_4}(R_0) \approx 10.5$, 6 and 5 for Ni^+, Pd^+ and Pt^+ in AgCl crystal. The structural data for md^9 octahedral clusters in AgCl are taken as $R_\perp = R_0$ and $R_{||} = R_0 + \Delta R$, where R_0 is the metal–ligand distance in AgCl and ΔR is the tetragonal elongation due to Jahn–Teller effect.

The molecular orbital coefficients N_γ, λ_γ and the ground overlap integrals $S_{dp}(\gamma)$ can be related by the normalization relationship obtained from Eq. (1), i.e.,

$$N_\gamma(1 + 2\lambda_\gamma S_{dp}(\gamma) + \lambda_\gamma^2) = 1 \quad (7)$$

So, if the coefficients λ_γ are known, the normalization coefficients N_γ can be calculated. In order to decrease the number of adjustable parameter, we assume $\lambda_t \approx \lambda_e \approx \lambda_\gamma$. Thus, in the above formulas, there are three unknown or adjustable parameters λ_γ, ΔR and κ. These parameters are determined by fitting the calculated spin-Hamiltonian parameters using the above formulas to the experimental values and the results for md^9 ions in AgCl are known in Table 1 (*note*: for Ni^+ in AgCl, there is no need for the fitting calculation of constants A_i because no observed values were reported. So, two adjustable parameters λ_γ and ΔR are required). The coefficients N_γ calculated from the values of λ_γ are also shown in Table 1 and then the parameters in Eq. (2) can be obtained from these coefficients. They are collected in Table 2. The calculated spin-Hamiltonian parameters are compared with the experimental values in Table 3.

3. Discussion

The sign of hyperfine structure constants A_i are related to the sign of constant P_0 and hence to the sign of nuclear magnetic moment μ_I [19,21,38]. The different signs of P_0 ($^{105}Pd^+$) and P_0 ($^{195}Pt^+$) suggest that the signs of constants A_i for AgCl:Pd^+ should differ from those for AgCl:Pt^+. It is difficult to determine the signs of constants A_i only by EPR experiment [19,21,39], so the observed values of constants A_i in many papers (including that for AgCl:Pt^+ given in Ref. [5]) obtained from EPR experiments are actually the absolute values although they are often written as positive values. Our calculations show that the signs of constants A_i for AgCl:Pd^+ are positive and those for AgCl:Pt^+ are negative. For AgCl:Pt^+, only the experimental value of $A_\perp$ has been reported, so the calculated value of $A_{||}$ in Table 3 remains to be cheeked by the further experimental study.

From a number of studies for the hyperfine structure constants A_i of md^n ions in the same crystal, a trend that the core polarization constant κ increases with the increase of m is found [33,34,37,40]. The values of κ for md^9 ions in AgCl crystals obtained from the above calculations are in keeping with the trend and can be regarded as reasonable.

It is noted that the potential energy surface for the Jahn–Teller distortion along the tetragonal axes has three minima. At low temperature, the md^9 ion is in one of the potential wells (i.e., static Jahn–Teller effect), which results in the anisotropic spin-Hamiltonian parameters. At high temperature, the higher vibrational states are populated and the md^9 ion converts rapidly from one state into another. The dynamic Jahn–Teller effect leads the spin-Hamiltonian parameters to be a mean value of those along three tetragonal axes and so they are isotropic, i.e.,

$$g_{iso} = \tfrac{1}{3}(g_{||} + 2g_\perp), \quad A_{iso} = \tfrac{1}{3}(A_{||} + 2A_\perp) \quad (8)$$

The isotropic g value of AgCl:Pd^+ at high temperature ($T \approx 293$ K) was measured [6]. Our calculated value of g_{iso} is very close to the observed value (see Table 3, the small difference of g_{iso} between calculation and experiment may be due to the fact that in the calculations the vibrational contribution to spin-Hamiltonian parameters [41–43] is neglected). The rest isotropic spin-Hamiltonian parameters (i.e., A_{iso} for AgCl:Pd^+, and g_{iso} and A_{iso} for AgCl:Pt^+) were not reported and also remain to be checked by experiments.

Table 3 shows that by using the high-order perturbation formulas based on the cluster approach with the suitable parameters, the spin-Hamiltonian parameters for the tetragonal md^9 centers in AgCl crystal are explained reasonably and the tetragonal elongations due to the static Jahn–Teller effect of these md^9 centers are obtained. It appears that the high-order perturbation formulas based on the cluster approach are effective to the calculation of spin-Hamiltonian parameters for md^9 ions in crystals.

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