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Citation: *The Journal of Chemical Physics* **79**, 4996 (1983); doi: 10.1063/1.445593

View online: <http://dx.doi.org/10.1063/1.445593>

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# A charge-transfer contribution to the $g_{\parallel}$ shift of $d^7$ ions in strong field situations

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(Received 24 February 1983; accepted 25 April 1983)

It is shown here that a good insight into the  $g_{\parallel}$  shift of  $d^7$  ions in elongated  $D_{4h}$  symmetry requires one to go beyond the crystal field approach and consider the levels arising from a molecular orbital picture. Within this scheme is demonstrated the appearance of a second order contribution to the  $g_{\parallel}$  shift which depends on the spin-orbit coefficient and the covalency of equatorial ligands. This new contribution can reasonably account for the positive  $g_{\parallel}$  shift observed for  $\text{Pd}^{3+}$  and  $\text{Rh}^{2+}$  doped silver halides. Furthermore, the smallness of the spin-orbit coefficient of equatorial ligands in cases such as  $[\text{Rh}(\text{CN})_4\text{Cl}_2]^{3-}$  or  $[\text{Fe}(\text{CN})_4\text{Cl}_2]^{5-}$  is consistent with the slightly negative  $g_{\parallel}$  shift observed for these systems.

## INTRODUCTION

In recent years several  $d^7$  ions doped into ionic lattices (and specially silver halides) have been investigated through the EPR technique.<sup>1-10</sup> Such studies have shown the existence of  $d^7$  systems in strong field situations displaying an elongated tetragonal geometry (Fig. 1). In those systems the spin of the ground state is  $S = \frac{1}{2}$ , the unpaired electron being placed on an orbital transforming like  $3z^2 - r^2$  (Fig. 2). The experimental  $g$  tensor of these systems has been analyzed through a theoretical crystal field approach, though empirical reduction factors have been allowed in order to take into account the covalency with nearest anions.<sup>4,5,8,10</sup>

The main goal of this work is to show that the existence of covalency in these systems can also give rise to the appearance of new contributions to the  $g$  tensor which cannot be obtained within a crystal field approach but only in a more realistic molecular orbital (MO) description of the  $[\text{MX}_6]$  cluster ( $\text{M} = d^7$  impurity,  $\text{X} = \text{halide}$ ). Furthermore, it is argued in this work that such contributions can be of great importance for understanding the experimental positive  $g_{\parallel}$  shift observed in  $\text{Rh}^{2+}$  and  $\text{Pd}^{3+}$  doped silver halides. In this way Table I points out that though  $g_{\perp} - g_0$  is rather similar for  $\text{Rh}^{2+}:\text{AgCl}$  and  $\text{Rh}^{2+}:\text{AgBr}$ , and the same happens for  $\text{Pd}^{3+}$  doped silver halides, significant differences appear in  $g_{\parallel} - g_0$ . For instance,  $g_{\parallel} - g_0$  is about three times higher for  $\text{Rh}^{2+}:\text{AgBr}$  than for  $\text{Rh}^{2+}:\text{AgCl}$ . This "anomalous" behavior, which up to now has not been explained, is not observed, e.g., for a  $d^9$  ion with an elongated  $D_{4h}$  geometry in which the values of both  $g_{\parallel} - g_0$  and  $g_{\perp} - g_0$  are comparable when  $\text{Br}^-$  is substituted by  $\text{Cl}^-$  as ligand.<sup>5,7,11</sup> Furthermore, in these cases the experimental  $g_{\parallel} - g_0$  and  $g_{\perp} - g_0$  values related to the  $[\text{MBr}_6]$  complex ( $\text{M} = \text{impurity ion}$ ) are slightly smaller than in the case of  $[\text{MCl}_6]$ . This fact is related to the slightly higher covalency of the  $[\text{MBr}_6]$  system which ultimately reflects the slightly smaller electronegativity of bromine compared to that of chlorine. This behavior is also observed when the experimental values of  $g_{\perp} - g_0$  of  $\text{Rh}^{2+}$  or  $\text{Pd}^{3+}$  doped  $\text{AgCl}$  are compared with the corresponding values for  $\text{Rh}^{2+}$  or  $\text{Pd}^{3+}$  in  $\text{AgBr}$  (Table I).

One key point of the present analysis lies in the fact

that for the present cases the crystal field scheme predicts  $g_{\parallel} - g_0 = 0$  at second order while

$$g_{\perp} - g_0 = 6\xi/\Delta, \quad (1)$$

where  $\xi$  is the spin-orbit coefficient of the central ion and  $\Delta$  is shown in Fig. 2.

Owing to this if the nonbonding levels of the  $[\text{MX}_6]$  complex give rise to a nonzero second order contribution to the  $g_{\parallel}$  shift it is clear that such a contribution can be very important for understanding the experimental  $g_{\parallel}$  shift of these systems.

It is now worthwhile to remark that for the present case crystal field theory predicts

$$g_{\parallel} - g_0 = -3\xi^2/\Delta^2 \quad (2)$$

at third order perturbations, so it implies a slightly negative  $g_{\parallel} - g_0$  value which anyway is at variance with the positive  $g_{\parallel}$  shift observed for  $\text{Rh}^{2+}$  and  $\text{Pd}^{3+}$  doped silver halides.

## THEORETICAL

Within a MO description the unpaired electron is placed on the  $a_{1g}^*$  one-electron orbital whose wave function can be written as

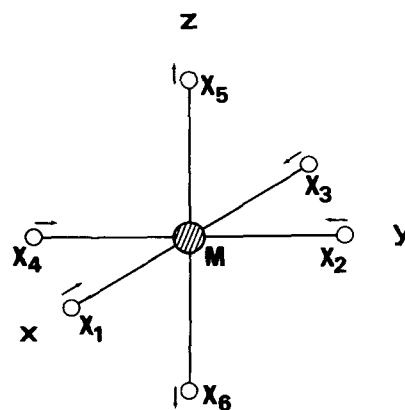


FIG. 1. Arrangement of the six ligands  $X$  around the  $d^7$  ion in an elongated  $D_{4h}$  symmetry. The arrow indicates the displacement of the ligands with respect to the octahedral geometry.

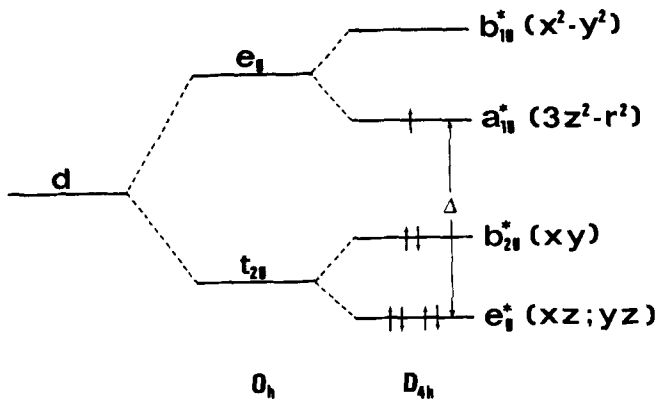


FIG. 2. Arrangement of the mainly  $d$  levels for a  $d^7$  impurity in an elongated  $D_{4h}$  symmetry. The irreducible representation to which the levels belong is indicated through Mulliken's notation. In a strong field situation the unpaired electron is placed in the  $a_{1g}$  orbital.

$$|a_{1g}^*\rangle = \alpha |d_{3z^2-r^2}\rangle - \beta \{ \mu |\chi_p^{ax}\rangle + (1 - \mu^2)^{1/2} |\chi_s^{ax}\rangle \} - \gamma \{ \nu |\chi_p^{eq}\rangle + (1 - \nu^2)^{1/2} |\chi_s^{eq}\rangle \}, \quad (3)$$

where

$$\begin{aligned} |\chi_p^{ax}\rangle &= \frac{1}{2} \{ -|p_x(5)\rangle + |p_x(6)\rangle \} \\ |\chi_s^{ax}\rangle &= \frac{1}{2} \{ |s(5)\rangle + |s(6)\rangle \} \\ |\chi_p^{eq}\rangle &= \frac{1}{2} \{ -|p_x(1)\rangle - |p_y(2)\rangle + |p_x(3)\rangle + |p_y(4)\rangle \} \\ |\chi_s^{eq}\rangle &= \frac{1}{2} \{ |s(1)\rangle + |s(2)\rangle + |s(3)\rangle + |s(4)\rangle \}. \end{aligned} \quad (4)$$

Here the  $|p_i(k)\rangle$  and  $|s(k)\rangle$  wave functions ( $i = x, y, z$ ;  $k = 1 \dots 6$ ) correspond to the valence orbitals of the six involved ligands.

Taking into account Stone's formula,<sup>12</sup> the second order contributions to  $g_{\parallel} - g_0$  are mainly controlled by virtual excitations in which either the unpaired electron goes to an empty orbital  $|e\rangle$  or an electron goes from an occupied orbital  $|O\rangle$  to the  $|a_{1g}^*\rangle$  orbital. The matrix elements which govern these processes are of the form  $\langle a_{1g}^* | T_x | n \rangle$  where  $T_x$  is an operator transforming like  $L_x$  and  $|n\rangle$  is either  $|e\rangle$  or  $|O\rangle$ . As  $L_x$  transforms as  $A_{2g}$  in  $D_{4h}$  that means that only whether  $|e\rangle$  or  $|O\rangle$  belong to  $A_{2g}$   $\langle a_{1g}^* | T_x | n \rangle$  will not be zero.

This simple argument thus explains why  $g_{\parallel} - g_0$  is zero at second order within a crystal field picture and at the same time shows that a nonbonding  $A_{2g}$  level will give rise to a nonzero second order contribution to  $g_{\parallel} - g_0$ .

In the present scheme there exists only one  $a_{2g}$  orbital which comes from the  $t_{1g}$  nonbonding level in  $O_h$  symmetry. The wave function of this  $a_{2g}$  level, built up only from equatorial ligands, is given by

$$|a_{2g}\rangle = \frac{1}{2} \{ |p_y(1)\rangle - |p_x(2)\rangle - |p_y(3)\rangle + |p_x(4)\rangle \}. \quad (5)$$

The spin-orbit coupling is given by  $T \cdot S$  where  $T$  is an operator transforming like  $L$  and given by<sup>12-14</sup>

$$T = \xi_M(r)L + \sum_{k=1}^6 \xi_L(r - r_k)L_k. \quad (6)$$

Here  $\xi_M(r)$  corresponds to the central ion while  $\xi_L(r - r_k)$  is related to the ligand placed at  $r_k$ .  $L_k$  means the or-

bital angular momentum referred to the position of the  $k$  ligand as origin.

Thus, following Stone's formula we can express the second order contribution to the  $g_{\parallel}$  shift for the present case, denoted as  $\Delta g_{\parallel}$ , as follows:

$$\Delta g_{\parallel} = 2 \langle a_{1g}^* | T_x | a_{2g} \rangle \langle a_{2g} | L_x | a_{1g}^* \rangle / \delta, \quad (7)$$

where  $\delta$  means  $\epsilon(a_{1g}) - \epsilon(a_{2g})$ .

Now taking into account that as  $\xi_L(r - r_k) \approx (r - r_k)^{-3}$ ,  $\xi_L(r - r_k)$  only connect in practice two atomic orbitals centered on the same atom,<sup>12-14</sup> we derive the following second-order expression for  $g_{\parallel} - g_0$ :

$$\Delta g_{\parallel} = 2\gamma^2 \nu \Gamma(\nu) \xi_L / \delta, \quad (8)$$

where  $\xi_L$  is the ligand spin-orbit coefficient while  $\Gamma(\nu)$  is given by

$$\Gamma(\nu) = \nu - (1 - \nu^2)^{1/2} R_{eq} \langle s | \frac{\partial}{\partial y} | p_y \rangle, \quad (9)$$

where  $R_{eq}$  is the equatorial metal-ligand distance and the atomic integral  $\langle s | \partial/\partial y | p_y \rangle$  has a value close to  $0.8 (\text{\AA})^{-1}$  for chlorine and bromine.<sup>15</sup> This factor  $\Gamma(\nu)$  depending on the ligand hybridization is thus responsible for the sign of the charge-transfer contribution  $\Delta g_{\parallel}$  given by Eq. (8). It should be recalled here that such a factor appears in the theoretical treatment of the  $g$  tensor of several impurities<sup>14-16</sup> and defects<sup>17</sup> within a MO approach. In particular it plays a key role for understanding the  $g$  shift of  $s^1$  impurities in  $O_h$  symmetry.<sup>16</sup>

Therefore, Eq. (8) tell us that, provided the third order contribution to  $g_{\parallel} - g_0$  be negligible, the sign of this quantity will be positive if  $\Gamma(\nu) > 0$ , a fact which is favored for small values of the  $s$ - $p$  ligand hybridization.

## APPLICATIONS, DISCUSSION

In this section we analyze the reliability of the mechanism described in the previous section in order to explain the experimental  $g_{\parallel}$  shift of  $Rh^{2+}$  and  $Pd^{3+}$  doped silver halides.

Taking  $\langle s | \partial/\partial y | p_y \rangle = 0.8 (\text{\AA})^{-1}$ , Eq. (8) indicates that the present mechanism will give rise to a positive contribution to  $g_{\parallel} - g_0$  only if  $\nu$  is higher than 0.90 provided  $R_{eq}$  be smaller than  $3 \text{\AA}$ . On the other hand, Eq. (8) clearly points out the linear dependence of  $\Delta g_{\parallel}$  with  $\xi_L$ . As  $\xi_L(\text{Br})/\xi_L(\text{Cl}) \approx 4$  we would expect a similar increase on  $\Delta g_{\parallel}$  when passing from  $[MCl_6]$  to  $[MBr_6]$  provided the equatorial covalency be similar in both systems. Therefore, this argument appears to explain to a great extent the "anomalous" increase of  $g_{\parallel} - g_0$  observed on going

TABLE I. Experimental values of  $g_{\parallel}$  and  $g_{\perp}$  for  $Rh^{2+}$  and  $Pd^{3+}$  doped silver halides;  $g_0$  is 2.0023.

	$10^3 (g_{\parallel} - g_0)$	$10^3 (g_{\perp} - g_0)$	Reference
$Rh^{2+}$ : Ag Cl	9	420	1
$Rh^{2+}$ : Ag Br	28	357	2
$Pd^{3+}$ : Ag Cl	10	182	5
$Pd^{3+}$ : Ag Cl	18	162	6
$Pd^{3+}$ : Ag Br	54	150	7

from  $\text{Pd}^{3+}:\text{AgCl}$  or  $\text{Rh}^{2+}:\text{AgCl}$  to  $\text{Pd}^{3+}:\text{AgBr}$  or  $\text{Rh}^{2+}:\text{AgBr}$ . Nevertheless, a quantitative comparison with the experimental results is not simple at present because in the EPR spectra only the superhyperfine (shf) interaction with axial ligands is resolved.<sup>1,2,5-7</sup> This fact reflects a stronger overlap of the  $d_{3z^2-r^2}$  metal wave function with the axial rather than with the equatorial ligands in spite of an equatorial metal-ligand distance  $R_{\text{eq}}$  shorter than the axial one  $R_{\text{ax}}$ .

Anyway, if we take the case of  $\text{Pd}^{3+}:\text{AgBr}$ <sup>7</sup> as a guide the analysis of the experimental shf tensor gives  $\beta = 0.64$ ,  $\mu = 0.97$ . Thus, if we assume that  $\nu$  is equal or close to  $\mu$  this value  $\nu = 0.97$  would lead to a positive  $\Delta g_{\parallel}$  contribution. In the case that  $R_{\text{eq}} = R_{\text{ax}}$  it should be verified that  $\beta = \sqrt{2}\gamma$ . Though in  $\text{Pd}^{3+}:\text{AgBr}$   $R_{\text{eq}}$  will be smaller than  $R_{\text{ax}}$  we shall take  $\gamma = 0.45$  as a first approximation. Moreover, assuming  $\nu = \mu = 0.97$ ,  $\delta = 25000 \text{ cm}^{-1}$ ,  $R = 2.9 \text{ \AA}$ , and taking  $\xi_L(\text{Br}) = 2456$  it is found that  $\Gamma = (\nu, R_{\text{eq}}) = 0.44$  and  $\Delta g_{\parallel} = 0.02$ , a value which is comparable to the experimental  $g_{\parallel}$  shift of  $\text{Pd}^{3+}:\text{AgBr}$ . On the other hand taking  $\Delta \approx 20000 \text{ cm}^{-1}$ ,<sup>7</sup>  $\xi(\text{Pd}^{3+}) = 1640 \text{ cm}^{-1}$ ,<sup>18</sup> and assuming a reduction factor of about 0.5 for this spin-orbit coefficient, the third order crystal field contribution is estimated to be around  $-6 \cdot 10^{-3}$ . Therefore, these figures support the idea that the present mechanism can actually be the main one responsible for the observed positive  $g_{\parallel} - g_0$  value in  $\text{Rh}^{2+}$  and  $\text{Pd}^{3+}$  doped silver halides. Moreover, as  $R_{\text{ax}} > R_{\text{eq}}$ , the actual value of  $\gamma$  should likely be higher than  $\beta/\sqrt{2}$ , a fact which would tend to increase the present theoretical estimation of the charge transfer contribution to the  $g_{\parallel}$  shift. Nevertheless, a more accurate calculation of the present contribution requires that one performs ENDOR experiments in order to measure the covalency parameters  $\gamma$  and  $\nu$  for the equatorial ligands.

It is now worthwhile to remark that charge transfer levels play a significant role in the interpretation of the experimental  $g$  shifts of other paramagnetic ions. In this sense, for instance, the positive  $g$  shift shown by  $\text{Fe}^{5+}$  doped  $\text{SrTiO}_3$  was ascribed to charge transfer excitations<sup>19</sup> which in this case play a dominant role likely because of the higher nominal charge of the involved cation. In this line it has been also shown<sup>16</sup> that the  $g$  shift of  $s^1$  ions in octahedral coordination in which crystal-field contributions are completely absent can be reasonably ascribed to the  $t_{1g} - a_{1g}^*$  charge transfer transition. A similar situation though more complex is encountered when dealing with high-spin systems of  $d^5$  ions. Here the work by Passegi, Kandel, and Buch<sup>20</sup> proves reasonably that the  $g$  shift of covalent complexes such as  $[\text{FeCl}_4]^-$  or  $[\text{FeBr}_4]^-$  has to be ascribed mainly to the admixture of excited charge transfer states having  $S = 5/2$  with the ground state via spin-orbit coupling.

Finally, in the case of  $d^9$  ions in a  $D_{4h}$  compressed geometry, it has been noted<sup>21</sup> that the small but negative  $g_{\parallel} - g_0$  shift of  $\text{Cu}^{2+}:\text{NH}_4\text{Cl}$  and  $\text{Cu}^{2+}:\text{NH}_4\text{Br}$  cannot be understood unless a charge transfer contribution similar to the present one be considered.

Anyway we believe that the experimental data on the  $[\text{Rh}(\text{CN})_4\text{Cl}_2]^{4-}$  complex in  $\text{KCl}^3$  supports quite well the present explanation for the  $g_{\parallel}$  shift of  $\text{Rh}^{2+}$  and  $\text{Pd}^{3+}$  doped

silver halides. In fact, while the axial shf tensor of that complex<sup>3</sup> is quite similar to that of  $\text{Rh}^{2+}$  doped  $\text{AgCl}$  or  $\text{NaCl}^1$  the  $g_{\parallel}$  shift is negative, its value being  $-0.007$  instead  $+0.009$  or  $+0.017$  as found in  $\text{Rh}^{2+}:\text{AgCl}$  or  $\text{NaCl}$ , respectively.<sup>1</sup> As in the  $[\text{Rh}(\text{CN})_4\text{Cl}_2]^{4-}$  complex the equatorial ligands are not chlorine but  $(\text{CN})^-$  ions, we should expect that the charge transfer contribution to the  $g_{\parallel}$  shift given by Eq. (8) would be about seven times smaller than in the case of  $\text{Rh}^{2+}:\text{AgCl}$  or  $\text{NaCl}$  mainly because  $\xi_L(\text{Cl})/\xi_L(\text{N}) = 7.7$ .

Therefore, this simple argument predicts that the present charge transfer contributions to the  $g_{\parallel}$  shift is practically negligible for the  $[\text{Rh}(\text{CN})_4\text{Cl}_2]^{4-}$  complex. Owing to this the experimental negative  $g_{\parallel} - g_0 = -0.007$  value found for  $[\text{Rh}(\text{CN})_4\text{Cl}_2]^{4-}$  is consistent with a dominant role of the third order crystal field contribution.

Quite recently, Viswanath and Rogers<sup>10</sup> have reported an extensive study about  $[\text{Fe}(\text{CN})_4\text{Cl}_2]^{5-}$  and  $[\text{Fe}(\text{CN})_4(\text{CN})\text{X}]^{5-}$  complexes ( $\text{X} = \text{Cl}, \text{Br}$ ) in alkali halide lattices. Such  $\text{Fe}(\text{I})$  complexes are of the same kind as those studied in the present work and they exhibit a  $g_{\parallel}$  shift which is again slightly negative (typically  $-0.004$ ).

In conclusion, though ENDOR measurements are desirable for measuring the equatorial covalency, it appears that the present mechanism can reasonably explain the origin of the  $g_{\parallel}$  shift of  $\text{Pd}^{3+}$  and  $\text{Rh}^{2+}$  doped silver halides.

It is clear that the present mechanism may have a minor role in the cases in which the involved  $d^7$  ion has a higher spin-orbit coefficient. This happens for instance for the  $5d^7$  ions  $\text{Ir}^{2+}$  ( $\xi = 4056 \text{ cm}^{-1}$ ) and  $\text{Pt}^{3+}$  ( $\xi = 5011 \text{ cm}^{-1}$ ).<sup>22</sup> In this sense the experimental results on  $\text{Ir}^{2+}$  doped  $\text{AgCl}$  and  $\text{AgBr}^8$  and  $\text{Pt}^{3+}:\text{AgCl}^9$  reveal a negative  $g_{\parallel}$  shift consistent with a dominant role of the third order crystal field contributions. Further work along this line is currently in progress.

## ACKNOWLEDGMENTS

We would like to thank Professor L. Slifkin, Professor M. T. Rogers, and Dr. R. S. Eachus for sending us copies of their recent work. Financial support by the "Comisión Asesora para la Investigación Científica y Técnica" is gratefully acknowledged.

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