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Molecular *g* Values of the $Cu(H_2O)_6^{2+}$ Ion

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The room-temperature EPR spectra of single crystals of $Cat_2Cu(SO_4)_2\cdot6H_2O$ [Cat = K, Rb, Tl, NH_4] and $K_2Cu(ZrF_6)_2\cdot6H_2O$ have been used to obtain the molecular *g* values of the $Cu(H_2O)_6^{2+}$ ion with a variety of different Cu–O bond lengths. Ground-state wave functions of the form $\psi \propto |cx^2 + ey^2 + fz^2\rangle$ have been derived for each compound, and the relationship between these and the structure of the copper complexes is discussed. In agreement with simple theory, there is an overall tendency for the Cu–O bond length to decrease as the magnitude of the parameter defining the ground-state lobe along the bond axis increases. However, the wave function parameters derived from the *g* values are generally considerably smaller than those calculated by the angular overlap simple molecular orbital bonding model. Possible explanations for this discrepancy in terms of temperature-dependent structural equilibria of $Cu(H_2O)_6^{2+}$ in the compounds are discussed.

Introduction

There has recently been considerable interest in the interpretation of molecular *g* values in terms of the ground-state wave functions of low-symmetry metal complexes.[1-4] The hexaaquocuprate(II) ions present in the copper Tutton salts [general formula $Cat_2Cu(SO_4)_2\cdot6H_2O$] (Cat = cation) provide a particularly useful series with which to test the relationships between EPR parameters and the electronic and molecular structure of metal complexes, as they contain complex ions having similar symmetries, but with a variety of different bond lengths.[5] Moreover, although the EPR spectra of several of these salts have been reported, the investigations were usually of a pioneering nature, and there has been little attempt to relate the *g* values to the molecular structures of the complexes.[6-8] In the present study, the molecular *g* values of the $Cu(H_2O)_6^{2+}$ ions in the K, NH_4, Rb, and Tl Tutton salts and $K_2Cu(ZrF_6)_2\cdot6H_2O$ have been measured by single-crystal EPR spectroscopy and used to deduce the ground-state wave functions in each complex. The way in which these are related to the molecular geometry of the hexaaquocuprate(II) ion is discussed.

Experimental Section

The preparation and morphology of single crystals of each complex have been described in the preceding paper. The EPR spectra of $(NH_4)_2Cu(SO_4)_2\cdot6H_2O$ and $K_2Cu(ZrF_6)_2\cdot6H_2O$ were measured using a JEOL JES-P-10 X-band spectrometer, while the spectra of the K, Rb, and Tl Tutton salts were obtained using an X-band Varian machine. The spectra run on the JEOL spectrometer were calibrated using a sample of ~0.5% Mn^{2+} doped into MgO, with the microwave frequency being measured using a standard reference cavity, while the Varian spectra were calibrated using DPPH, and a frequency meter was used to check the microwave frequency. All measurements were made at room temperature.

Spectra were measured by mounting crystals with well-developed faces on the bottom or side of a quartz rod using a stereoscopic microscope. This rod was mounted in a quartz EPR tube which was placed in a rotatable jacket having a calibrated scale attached to it. By this means the angles of rotation of each crystal plane relative to the applied static magnetic field *H* could be measured to ±1°. The EPR spectra were measured at regular intervals (usually 10°) for rotations of about 180° in the (010), (001), and *bc** (orthogonal to [100]) crystal planes of each compound. In general, the observed EPR signals were due to the superimposition of the resonances from the two inequivalent molecules in each unit cell (these being precisely coincident only when *H* was along, or perpendicular to, the *b* crystal axis[4]). The individual signals were only well enough resolved to be of value in the estimation of the molecular parameters in the (001) planes of the K, Rb, and Tl Tutton salts and $K_2Cu(ZrF_6)_2\cdot6H_2O$ and the *bc** plane of $(NH_4)_2Cu(SO_4)_2\cdot6H_2O$. Line-fitting procedures were used to accurately assign the position of the two peaks (though in fact only small corrections were required to overcome this problem). For rotations in crystal planes other than (010) the absolute position of *H* in the crystal could be determined accurately by making use of the fact that the signals from the two inequivalent molecules coalesced when *H* was along, or perpendicular to, the *b* crystal axis. For the rotations in the (010) plane of $(NH_4)_2Cu(SO_4)_2\cdot6H_2O$ and $K_2Cu(ZrF_6)_2\cdot6H_2O$, the position of *H* relative to the crystal coordinates was determined from the known values of *g* with *H* along *a* and *c** obtained from the rotations in the other two planes. For the K, Rb, and Tl salts this was not feasible, as in the (010) plane g^2 showed only a slight variation as a function of angle in the region of the *a* and *c** axes. Hence, for these latter complexes, only data from the (001) and *bc** rotations was used in the calculation of the molecular *g* values, with the crystal being independently mounted at least twice for each rotation. The method used to calculate the molecular *g* values has been given elsewhere.[2,4] The data used in the calculations are given in Table I (supplementary material), and the molecular *g* values obtained for each complex are shown in Table II. Because of the comparatively limited experimental data, the principal *g* axes were assumed to be coincident with the molecular axes defined as in the preceding paper, i.e., with *x* along the shortest Cu–O bond direction and *y* and *z* along the intermediate and longest Cu–O bonds, respectively. Accurate molecular *g* values were previously available only for the NH_4 Tutton salt, which was studied by Mabbs and Porter at "Q"-band frequency.[8] These workers found the principal molecular *g* axes to lie very close to the Cu–O bond directions. The molecular *g* values of $(NH_4)_2Cu(SO_4)_2\cdot6H_2O$ obtained in the present study agree well with those reported by Mabbs and Porter (Table II).

Discussion

Derivation of the Ground-State Wave Functions from the *g* Values. Rigorously, the $Cu(H_2O)_6^{2+}$ ion in the Tutton salts belongs to the point group C_i[5], so that the metal part of the ground-state wave function in the absence of spin–orbit coupling consists of an admixture of all five d orbitals. In fact, the ligand field is composed of a dominant D_{4h} component, with an additional perturbation due to the inequivalent bond lengths along the *x* and *y* axes which lowers the point group to D_{2h} and a further lowering of the symmetry to C_i because of the nonplanarity of the atoms in each Cu–OH_2 unit. In the D_{4h} point group the metal part of the ground state is $d_{x^2-y^2}$, and the lowering of the symmetry to D_{2h} causes this to become contaminated with d_{z^2}. The further lowering of the symmetry to C_i is accompanied by a change in the nature of the interaction of the water molecules with the metal d_{xy}, d_{xz}, and d_{yz} orbitals and the consequent participation of these in the ground state. While the effects of the contamination of the ground state by d_{z^2} on the molecular *g* values are well established,[1-4,9] the results of an admixture of d_{xy}, d_{yz}, and d_{xz} have apparently not been considered previously. However, participation of these latter orbitals should have little effect on the *g* values. This is because contributions from this source always contain products of the molecular orbital coefficients of two of the minor components of the ground state (e.g., d_{z^2} and d_{xz}) multiplied by the normal perturbation term.[10] This contrasts with the effect of the admixture of d_{z^2} into the ground state, which yields a contribution to g_x and g_y which is linear in the coefficient of this orbital (see following equations). Moreover, in the case of the NH_4 salt, where the participation

Table II. Molecular *g* values and Bond Lengths of Compounds Containing the Hexaaquocuprate(II) Ion Measured at Room Temperature

Compd	*g* value[a]			Bond length, pm			Bond length ref
	x	*y*	*z*	*x*	*y*	*z*	
$(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$	2.071 (0.0015)	2.209 (0.012)	2.363 (0.020)	196.60	207.25	223.00	25
$(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$[b]	2.071 (0.001)	2.218 (0.000)	2.360 (0.002)				
$K_2Cu(SO_4)_2 \cdot 6H_2O$	2.0549 (0.0025)	2.1539 (0.001)	2.4027 (0.0025)	194.3	206.9	227.8	21
$Rb_2Cu(SO_4)_2 \cdot 6H_2O$	2.0737 (0.0049)	2.1090 (0.0014)	2.4201 (0.002)	195.7	203.1	230.7	23
$Tl_2Cu(SO_4)_2 \cdot 6H_2O$	2.0704 (0.0034)	2.1161 (0.0008)	2.4180 (0.0005)	195.7	201.7	231.7	24
$K_2Cu(ZrF_6)_6 \cdot 6H_2O$	2.0606 (0.0045)	2.1387 (0.0059)	2.4430 (0.0014)	196.7	202.4	232.7	26
Copper hydrogen maleate hexahydrate[c]	2.085 (0.001)	2.089 (0.001)	2.353 (0.001)	193.3	195.9	268.2	20

[a] Uncertainties are given in parentheses. [b] *g* values from ref 8. [c] *g* values from ref 4.

Table III. Ground State Wave Function Parameters of the Complexes

Compd	Wave function parameters derived from *g* values[a]			Calcd parameter,[b] *f*	Reduction parameters[c]	
	c	*e*	*f*		$k_\perp$	$k_\parallel$
$(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$	1.860 (8)	−1.566 (10)	−0.294 (10)	−0.476 (12)	0.97 (2)	0.77 (2)
$K_2Cu(SO_4)_2 \cdot 6H_2O$	1.853 (20)	−1.579 (25)	−0.275 (30)	−0.460 (14)	0.86 (2)	0.78 (2)
$Rb_2Cu(SO_4)_2 \cdot 6H_2O$	1.778 (20)	−1.682 (25)	−0.097 (30)	−0.258 (20)	0.82 (2)	0.80 (2)
$Tl_2Cu(SO_4)_2 \cdot 6H_2O$	1.794 (20)	−1.664 (25)	−0.130 (30)	−0.206 (32)	0.83 (2)	0.80 (2)
$K_2Cu(ZrF_6)_2 \cdot 6H_2O$	1.835 (30)	−1.607 (30)	−0.228 (45)	−0.196 (40)	0.86 (2)	0.81 (2)
Copper hydrogen maleate hexahydrate[d]	1.738 (1)	−1.726 (1)	−0.012 (2)	−0.029 (4)	0.83 (1)	0.93 (1)

[a] Errors in parentheses × 10^{-3}. [b] Calculated using the angular overlap model; see text for method. [c] Errors in parentheses × 10^{-2}. [d] Data from ref 4.

of d_{xy} etc. would probably be at a maximum, it is known that the principal *g* axes coincide quite closely with the bond directions. Direct participation of the metal "π" orbitals in the ground state should cause a rotation of the *g* axes away from the bond directions. It therefore seems safe to neglect the participation of d_{xy}, d_{xz}, and d_{yz} in the ground-state wave function, the metal part of which may thus be written $\psi = |ad_{x^2-y^2} - bd_{z^2}\rangle$, where $a^2 + b^2 = 1$. The equations for the *g* shifts are those for a complex of D_{2h} symmetry[9]

$$\Delta g_x = \frac{-2\lambda}{E_{yz}} k_1{}^2 (a - 3^{1/2} b)^2 \qquad (1a)$$

$$\Delta g_y = \frac{-2\lambda}{E_{xz}} k_2{}^2 (a + 3^{1/2} b)^2 \qquad (1b)$$

$$\Delta g_z = \frac{-8\lambda}{E_{xy}} a^2 k_3{}^2 \qquad (1c)$$

where E_i represents the energy of the excited state in which the unpaired electron occupies the orbital denoted by the subscript, λ is the spin–orbit coupling constant (−828 cm^{-1} for Cu^{2+}), and k_1, k_2, k_3 are orbital reduction parameters.[11] The net effect of the admixture of d_{z^2} into the ground state is to produce a new wave function of the form $\psi = |cx^2 + ey^2 + fz^2\rangle$ with unequal lobes along *x*, *y*, and *z*, where

$$c = b + 3^{1/2} a \qquad (2a)$$

$$e = b - 3^{1/2} a \qquad (2b)$$

$$f = -2b \qquad (2c)$$

The expression of the ground-state wave function in this manner has proved particularly useful where a correlation with molecular geometry is of interest.[3,4] The parameters *c*, *e*, and *f* were calculated from the molecular *g* values of each complex using an iterative procedure[4] and the results are listed in Table III. The excited-state energies were those obtained from the polarized spectra of the complexes.[12] The parameters were calculated with the restriction $k_1 = k_2 = k_\perp$, $k_3 = k_\parallel$. As the assumption of axial symmetry in the orbital reduction parameters might be invalid in these complexes, the effect of varying the ratio $k_1{:}k_2$ over a reasonable range was also investigated, and the results have been incorporated in the uncertainties in the wave function parameters.

Correlation of the Wave Function Parameters with Molecular Structures. There has been considerable interest in the interpretation of the molecular structures of six-coordinate copper(II) complexes in terms of the Jahn–Teller theorem.[13–15] It has been pointed out[15] that, strictly speaking, this theorem is applicable only for the comparatively rare complexes involving six identical ligands. There is apparently a delicate balance between the various structures which could be adopted by a complex of this kind. For instance, the hexanitrocuprate(II) ion has an elongated tetragonal structure in $K_2CaCu(NO_2)_6$,[16] and a regular octahedral structure, though probably accompanied by a dynamic Jahn–Teller distortion, in $K_2PbCu(NO_2)_6$ at room temperature,[17,18] while in $Rb_2PbCu(NO_2)_6$ the anion has been reported to have a compressed tetragonal structure.[13] However, it has recently been suggested[18,19] that in this last compound, the apparent appearance of a compressed tetragonal structure is in fact due to a dynamic equilibrium between ions having the more usual elongated tetragonal configuration. The hexaaquocuprate(II) ion also exhibits a range of structures, from that of a highly elongated tetragonal geometry in copper hydrogen maleate[20] through the rhombically distorted ions with three quite different bond lengths in the Tutton salts[21–25] and $K_2Cu(ZrF_6)_2 \cdot 6H_2O$[26] to the regular octahedral ion (though with a dynamic distortion) observed in $Cu(SiF_6) \cdot 6H_2O$.[14] Clearly, factors such as the size and bonding capacity of the countercation and intermolecular hydrogen bonding tend to have a dominant influence on the geometry of complexes of this kind. It is also generally recognized[27] that there is a relationship between the asymmetry of the d-electron density and the molecular structure of these complexes, with shorter bond lengths being associated with the directions of the ground-state lobes containing the unpaired electron. While this relationship is well established for the elongated and compressed tetragonal structures having ground states composed of a single d orbital, little attention has been paid until recently to the way in which the ground-state wave function is related to the molecular structure in a complex with rhombic symmetry. The use of a ground-state wave function of the form $|cx^2 + ey^2 + fz^2\rangle$ is particularly convenient in considerations of this kind, as the complete range of compounds can be described using a common coordinate system.[3] In a centrosymmetric compound of general formula $CuL_6{}^{2+}$ having axial symmetry, with four short bonds defining the *x* and *y* axes and two long bonds along

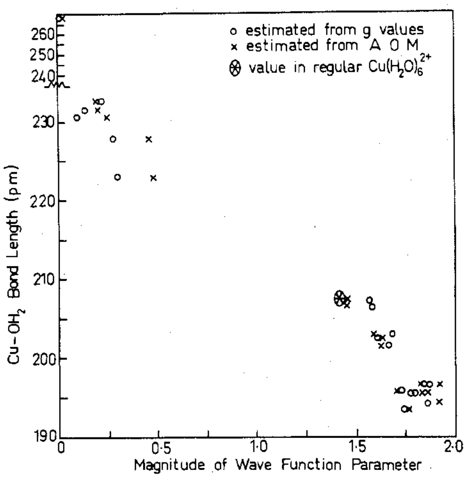

Figure 1. Relationship between the bond length and the extent of the ground-state lobe along the bond direction, as estimated from the molecular g values and calculated using the angular overlap model.

z, the ground-state wave function parameters are $c = 3^{1/2}$, $e = -3^{1/2}$, and $f = 0.0$. If the ligands along x and z move closer to the metal, while the bond lengths along y increase, giving a complex with rhombic symmetry, simple theory suggests that c should increase, while e should decrease, and f will become nonzero. If this process continues until the bonds along y and z are identical, the final wave function parameters become $c = 2$ and $e = f = -1$ and the complex again has axial symmetry, though with the unique axis labeled x rather than the more conventional z. The variation of the molecular g values accompanying a distortion of this kind has been discussed in detail elsewhere.[3] A dynamic Jahn–Teller distortion, producing a regular octahedral geometry when averaged, can be described by a wave function in which the parameters c, e, and f are time dependent, with average magnitudes $|c| = |e| = |f| = 2^{1/2}$.

Inspection of the values listed in Tables II and III shows that, in agreement with simple theory, there is an inverse correlation between the magnitude of the wave function parameter and the associated bond length for the $Cu(H_2O)_6^{2+}$ ion in each of the compounds studied here; i.e., the stronger the ligand σ perturbation, the larger the magnitude of the ground state wave function parameter. This lends support to the studies which have suggested that in centrosymmetric complexes with different ligands at similar distances along x and y, the wave function parameter of larger magnitude is associated with a greater ligand σ perturbation.[4,28] The overall relationship between the bond lengths and the magnitudes of the wave function parameters for the complexes as a whole is illustrated in Figure 1. The Cu–O distance in the regular $Cu(H_2O)_6^{2+}$ ion present in $Cu(SiF_6)\cdot 6H_2O$ is included in the diagram. While there is considerable scatter in the points, it is apparent that there is a general tendency for the Cu–O bond length to shorten as the magnitude of the wave function parameter along that direction increases. It is of interest to note that the empty region of the graph, between wave function parameters 0.5 and 1.4 and bond lengths 210 and 220 pm, corresponds to a geometry close to that of the compressed tetragonal structure having axial symmetry. This geometry would seem to be comparatively unstable for the $Cu(H_2O)_6^{2+}$ ion.

The wave function parameters derived from the g values may be compared with those calculated using the simple angular overlap model (AOM) developed by Jorgensen and Schäffer.[29] Here, the interaction between the metal and ligand orbitals is related to the square of the diatomic overlap integral, summed over all of the ligands in the complex, with the mixing coefficient b being given by the eigenvectors of the 2 × 2 matrix produced by the σ bonding of the water molecules with $d_{x^2-y^2}$ and d_{z^2}.[29] The calculated value of f for each complex is given in Table III (the other wave function parameters are easily obtained from the expressions in eq 2 and are shown in Figure 1). For the four Tutton salts, while the *relative* values of the mixing coefficients from the g values agree fairly well with the calculated values (those for the Rb and Tl salts being about half those found for the more rhombically distorted K and NH_4 salts), the calculated value is in each case approximately twice that obtained from the EPR spectra (Table III). Only for $K_2Cu(ZrF_6)_2\cdot 6H_2O$ is there good agreement between the calculated and experimental values. Possibly, the superficial treatment of covalency in the present study might contribute to the discrepancies; however, it seems most unlikely that this neglect could introduce any large error in compounds of this kind.[30] The assumption which is more likely to be suspect is that the measured g values may be directly related to the observed molecular structures of the Tutton salts. It is known that at least in the case of the NH_4 Tutton salt the EPR spectra show a marked change when the temperature is lowered.[8] At 160 K the $Cu(H_2O)_6^{2+}$ in this salt has molecular g values of 2.076, 2.131, and 2.433[8] corresponding to wave function parameters of $c = 1.801$, $e = -1.653$, and $f = -0.148$. A similar decrease in the rhombic nature of the molecular susceptibility tensor of the $Cu(H_2O)_6^{2+}$ ion has been observed in the K and NH_4 Tutton salts.[31] Mabbs and Porter attributed the change in the g values to an alteration in the nature of the π bonding between the copper ion and the water molecules.[8] However, the rhombic component of the g tensor is dominated by the admixture of d_{z^2} into the ground state and this admixture is related to the difference in σ bonding with the water molecules along the x and y axes (see preceding paper for the relevant matrix element). It therefore seems far more likely that, as has been suggested by Marshall,[31] the change in the g values with decreasing temperature is associated with an alteration in the bond lengths in the $Cu(H_2O)_6^{2+}$ unit. The electronic spectra suggest a slight decrease in the tetragonality as the temperature is lowered (see preceding paper) while the molecular g values indicate a smaller difference in σ bonding along the x and y axes than that suggested by the room-temperature structure determination. The overall implication of the EPR and electronic spectral data is therefore that at low temperatures the $Cu(H_2O)_6^{2+}$ ions in the Tutton salts have geometries with the bonds along x and y more nearly equal and the bond along z somewhat longer than those measured at room temperature. In the case of the ammonium salt, the data at low temperature are consistent with a shortening of the bond along y by ~2 pm and a lengthening of those along x and z by ~2 and ~8 pm, respectively, compared with the values of Cu–O = 196.6, 207.25, and 223.0 pm measured at room temperature.[32]

There would seem to be two possible explanations for the temperature variation of the g values and the discrepancy between the wave function parameters obtained from the EPR results and those estimated from the AOM calculations. First, as has been suggested by Marshall,[31] there could be a rapid dynamic equilibrium between two structural forms of the $Cu(H_2O)_6^{2+}$ ion, say A and B, both having the same orientation in the crystal lattice, with essentially similar geometries but with the lower energy form having a smaller rhombic distortion and consequently a smaller g anisotropy than the higher energy form. At any temperature the measured g value would then be given by

$$g = n_A g_A + n_B g_B$$

where n represents the fraction of molecules having the structure denoted by the subscript. If the structure measured at room temperature is closer to the higher energy form than is warranted by the fractions n_A and n_B, then a discrepancy between the measured g values and the structure-based calculations is to be expected. Some support for this hypothesis is provided by the plot of the wave function parameters calculated by the AOM against the corresponding bond lengths, which shows a more regular correlation than do the parameters estimated from the g values, as well as good agreement with the average bond length in the regular hexaaquocuprate(II) ion. A second possible explanation is that at room temperature a rapid, dynamic equilibrium occurs with a higher energy form of the $Cu(H_2O)_6^{2+}$ ion having molecular g values similar to those of the low-energy form but having the directions of the y and z molecular axes interchanged. The net effect of this would be to cause g_y and g_z to converge with increasing temperature, while leaving g_x essentially temperature independent, as is observed experimentally for $(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$ ($g_x = 2.076$, $g_y = 2.131$, $g_z = 2.433$ at 160 K; $g_x = 2.071$, $g_y = 2.218$, $g_z = 2.360$ at room temperature).[8] In agreement with this, the thermal parameters in the neutron diffraction study of $(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$ were found to be significantly greater for the oxygen atoms situated along the y and z directions than for those along the x direction.[25,33] Dynamic equilibria of this kind, corresponding to pseudorotations of the molecular axes in the crystal, are well established for the $Cu(H_2O)_6^{2+}$ ion in other systems.[34,35] For instance, a small amount of Cu^{2+} doped into $K_2Zn(SO_4)_2 \cdot 6H_2O$ has g values of $g_x = 2.03$, $g_y = 2.15$, and $g_z = 2.42$ at 20 K and $g_x = 2.02$, $g_y = 2.26$, and $g_z = 2.31$ at 295 K.[34] This has been explained by assuming that at the lower temperature the molecular axes of all of the crystallographically equivalent $Cu(H_2O)_6^{2+}$ ions are parallel, but as the temperature is raised, a rapid dynamic equilibrium takes place with a state $\sim 75\ cm^{-1}$ higher in energy in which the y and z axes and, presumably, the bond lengths along these directions are interchanged. It is interesting to note that the behavior of $Cu(H_2O)_6^{2+}$ in $K_2Zn(SO_4)_2 \cdot 6H_2O$ is rather different from that in the pure copper salt. While the g values of the former species at 20 K are similar to those of the latter at 295 K (Table II), the g values measured at the *same* temperature are quite different. This discrepancy in behavior presumably reflects the differing effects of the surrounding lattice upon the $Cu(H_2O)_6^{2+}$ ions in the two crystal environments. The present data would seem to be insufficient to determine which, if either, of the above mechanisms applies in the case of the pure copper Tutton salts. A detailed study of the temperature dependence of the g tensors of these compounds would be highly desirable, and we hope to carry out such a study in the near future. However, if either mechanism should prove correct, it emphasizes the fact that caution must be exercised in the correlation of spectral parameters with molecular structures, even when these have been measured at the same temperature; clearly, it is advisable to test the temperature dependence, particularly of EPR parameters, whenever this is possible.

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Registry No. $(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$(salt form), 13587-26-3; $(NH_4)_2Cu(SO_4)_2 \cdot 6H_2O$(coordinated form), 41584-35-4; $K_2Cu(SO_4)_2 \cdot 6H_2O$(salt form), 13587-29-6; $K_2Cu(SO_4)_2 \cdot 6H_2O$(coordinated form), 38797-50-1; $Rb_2Cu(SO_4)_2 \cdot 6H_2O$(salt form), 21349-43-9; $Rb_2Cu(SO_4)_2 \cdot 6H_2O$(coordinated form), 40275-15-8; $Tl_2Cu(SO_4)_2 \cdot 6H_2O$(salt form), 20908-85-4; $Tl_2Cu(SO_4)_2 \cdot 6H_2O$(coordinated form), 39698-58-3; $K_2Cu(ZrF_6)_2 \cdot 6H_2O$, 59492-79-4.

Supplementary Material Available: Table I, showing measured g^2 values for various orientations of the magnetic field in single crystals of the complexes (1 page). Ordering information is given on any current masthead page.

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(12) See the preceding paper in this issue for the transition energies; in the case of E_{yz} which could not be assigned accurately for most of the complexes, the wave function parameters were calculated for the widest extremes likely for this transition energy.

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