

This article was downloaded by:

On: 24 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Journal of Coordination Chemistry

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713455674>

The EPR Spectra of Tetradentate Schiff-Base Complexes of Copper II V. N,N'-bis(1,1,1-trifluoro 2,4-hexanedione)1,2-propanediimine

Robert L. Lancione^{ab}; Harry C. Allen Jr.^a

^a Department of Chemistry, Jeppson Laboratory, Clark University, Worcester, Massachusetts, U.S.A. ^b New England Research, Inc., Worcester, Massachusetts, U.S.A.

To cite this Article Lancione, Robert L. and Allen Jr., Harry C.(1976) 'The EPR Spectra of Tetradentate Schiff-Base Complexes of Copper II V. N,N'-bis(1,1,1-trifluoro 2,4-hexanedione)1,2-propanediimine', *Journal of Coordination Chemistry*, 6: 2, 127 – 128

To link to this Article: DOI: 10.1080/00958977608079897

URL: <http://dx.doi.org/10.1080/00958977608079897>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

SHORT COMMUNICATION

The EPR Spectra of Tetradentate Schiff-Base Complexes of Copper II V. N,N'-bis(1,1,1-trifluoro 2,4-hexanedione)1,2-propanediimine[†]

ROBERT L. LANCIONE[‡] and HARRY C. ALLEN, Jr.

Department of Chemistry, Jeppson Laboratory, Clark University, Worcester, Massachusetts 01610, U.S.A.

(Received July 20, 1976)

KEYWORDS: EPR spectrum, N,N'-bis(1,1,1-trifluoro-2,4-hexanedione)-1,2-propanediimine, spin-Hamiltonian parameters, bonding

As a part of a continuing study¹⁻⁴ of the effect of ligand structure on the bonding in copper(II) Schiff-base complexes the EPR spectrum of N,N'-bis(1,1,1-trifluoro-2,4-hexanedione)-1,2-propanediimine copper(II), [Cu pn(tfhex)₂], has been studied.

The Ni(II) chelate was synthesized containing 1-3% ⁶³Cu by methods previously described^{1,5} and characterized by partial elemental analysis. Calculated: C -41.90%, H -3.98%, N -6.52%; Found: C -42.0%, H -4.16%, N -6.50%.

Single crystals of the Cu(II) doped Ni[pn(tfhex)₂], were grown by slow evaporation of acetone solution. The complex crystallized as hexagonal platelets. No x-ray crystallographic structure study of either the Ni(II) or Cu(II) complex has been done.

EPR spectra were recorded at angular increments of 10° in planes perpendicular to the axes shown in Figure 1. The data were reduced by standard techniques¹ to yield the parameters of the spin-Hamiltonian for a doublet spin state. The results are listed in Table I. Values for g_z and A_z determined from the spectrum of a polycrystalline sample are in excellent agreement with those determined from the single crystal measurements. Only one magnetic site was observed in the single crystal spectrum and for that site the z-axis of the g-tensor coincides with the z-axis in Figure 1. Because g_x and g_y, A_x and A_y are nearly equal it was not possible to locate the tensor axes precisely but they are believed to coincide with the x and y axes in Figure 1.

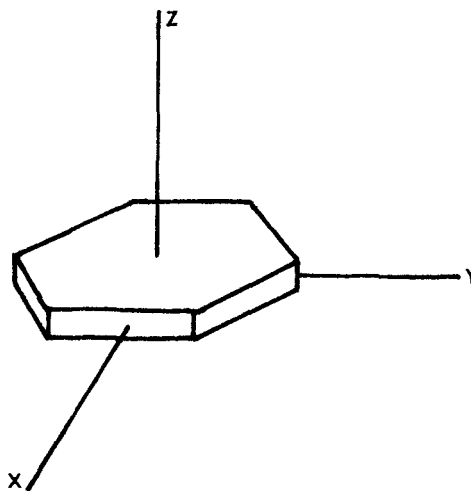


FIGURE 1 Relationship between crystal morphology and laboratory axis system.

The values of the magnetic parameters of [Cu(pn(tfhex)₂] are essentially the same as those obtained in the analysis of the EPR spectrum of N,N'-bis(trifluoro-2,4-hexanedione)ethylenediimine

TABLE I
Spin-Hamiltonian parameters for Cu[pn(tfhex)₂]

g _z	2.195 ± 0.001	
g _x	2.048 ± 0.002	
g _y	2.047 ± 0.002	
A _z ^{Cu}	193.3 ± 0.5 G	198.1 × 10 ⁻⁴ cm ⁻¹
A _x ^{Cu}	32.8 ± 1.0 G	31.4 × 10 ⁻⁴ cm ⁻¹
A _y ^{Cu}	31.9 ± 1.0 G	30.5 × 10 ⁻⁴ cm ⁻¹
A _z ^N	12.4 ± 0.5 G	12.7 × 10 ⁻⁴ cm ⁻¹
A _x ^N = A _y ^N	15.9 ± 0.5 G	15.2 × 10 ⁻⁴ cm ⁻¹

[†]Supported in part by the Bureau of Mines, Department of Interior under Contract PO 160064.

[‡]Present address: New England Research, Inc., 15 Sagamore Road, Worcester, Massachusetts 01605, U.S.A.

Cu(II) [Cu en(tfhex)₂] indicating that the change in the bridging amine in the Schiff-base ligand has minimal effect of the environment of the Cu(II) ion in the complex. Calculation of the wave function coefficients in the usual ligand field wave functions¹ showed them to be essentially the same for both chelates.

ACKNOWLEDGEMENTS

The authors wish to acknowledge the Lever Brothers Fund for summer support of one of us (R.L.L.) and the Research Corporation for an equipment grant.

REFERENCES

1. R. L. Lancione, H. C. Allen, Jr. and D. R. Sydor, *J. Coord. Chem.*, **4**, 153 (1975).
2. M. I. Scullane and H. C. Allen, Jr., *J. Coord. Chem.*, **4**, 255 (1975).
3. R. L. Lancione and H. C. Allen, Jr., *J. Coord. Chem.*, **4**, 261 (1975).
4. R. L. Lancione, H. C. Allen, Jr. and J. R. Buntaine, *J. Coord. Chem.*, (in press).
5. P. J. McCarthy, R. Hovey, K. Uneo and A. E. Martell, *J. Am. Chem. Soc.*, **77**, 5820 (1955).