

PARAMAGNETIC RESONANCE

PROCEEDINGS OF THE FIRST INTERNATIONAL
CONFERENCE HELD IN JERUSALEM, JULY 16-20, 1962

Edited by

W. LOW

Department of Physics

The Hebrew University of Jerusalem, Israel

Volume I

PARAMAGNETIC RESONANCE

PROCEEDINGS OF THE FIRST INTERNATIONAL
CONFERENCE HELD IN JERUSALEM, JULY 16-20, 1962

Edited by

W. LOW

Department of Physics

The Hebrew University of Jerusalem, Israel

Volume I



1963

ACADEMIC PRESS • NEW YORK • LONDON

Contributors to Volume II

Numbers in *italics* indicate the page on which the author's contribution appears.

- ROLAND AASA, Institute of Physics, University of Uppsala, Sweden (509)
 HIDERATO ABE, Institute of Solid State Physics, University of Tokyo, Azabu, Tokyo, Japan (557, 567, 587)
 A. G. ANDERSON, International Business Machines Research Laboratory, San Jose, California, U.S.A. (591)
 J. O. ARTMAN, Applied Physics Laboratory, The Johns Hopkins University, Silver Spring, Maryland, U.S.A. (634)
 J. M. ASSOUR, Radio Corporation of America, Princeton, New Jersey, U.S.A. (855)
 GEORGE W. BARTON, JR., Lawrence Radiation Laboratory, University of California, Livermore, California, U.S.A. (698)
 R. BATTUT, Laboratoire de Radioélectricité, Faculté des Sciences, Clermont-Ferrand, France (520)
 L. BELLOMONTE, Istituto di Fisica dell'Università, Palermo, Italy and Sezione Siciliana dell'Istituto Nazionale di Fisica Nucleare (790)
 G. B. BENEDEK, Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A. (696)
 H. BENOIT, Faculté des Sciences, Orsay (Seine et Oise), France (414)
 G. BERTHET, Laboratoire de Radioélectricité, Faculté des Sciences, Clermont-Ferrand, France (520)
 N. BLOEMBERGEN, Harvard University, Cambridge, Massachusetts, U.S.A. (607, 656)
 J. BROSEL, Laboratoire de Physique de l'Ecole Normale Supérieure, Paris, France (535)
 HARMON W. BROWN, Instrument Division, Varian Associates, Palo Alto, California, U.S.A. (704)
 M. E. BROWNE, Lockheed Research Laboratories, Palo Alto, California, U.S.A. (447)
 G. COLLINS, Department of Chemistry, University of California, Los Angeles 24, California, U.S.A. (496)
 A. CUNLIFFE, Department of Physics, The University of Hull, Hull, England (755)
 MUNEYUKI DATE, Department of Physics, Faculty of Science, Osaka University, Osaka, Japan (665)
 L. DE LAET, Instituut voor Lage Temperaturen en Technische Fysica, The Catholic University of Leuven, Leuven, Belgium (905)
 W. I. DOBROV, Lockheed Research Laboratories, Palo Alto, California, U.S.A. (447)
 J. EISINGER, Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A. (501)
 ELSA FEHER, University of California, La Jolla, California, U.S.A. (628)
 G. FEHER, University of California, La Jolla, California, U.S.A. (715)
 T. E. FEUCHTWANG, Department of Physics and Coordinated Science Laboratory, University of Illinois, Urbana, Illinois, U.S.A. (740, 749)
 G. F. J. GARLICK, Department of Physics, The University of Hull, Hull, England (755)
 T. GAROFANO, Istituto di Fisica dell'Università, Palermo, Italy, and Sezione Siciliana dell'Istituto Nazionale di Fisica Nucleare (582)
 GORDON L. GOODMAN, Argonne National Laboratory, Lemont, Illinois, U.S.A. (880)

- W. GORDY, Department of Physics, Duke University, Durham, North Carolina, U.S.A. (795)
- J. GRENIER, Laboratoire de Radioélectricité, Faculté des Sciences, Clermont-Ferrand, France (520)
- F. S. HAM, General Electric Research Laboratory, Schenectady, New York, U.S.A. (620)
- E. A. HARRIS, Clarendon Laboratory, Oxford, England, (553)
- S. E. HARRISON, Radio Corporation of America, Princeton, New Jersey, U.S.A. (855)
- S. R. HARTMAN¹, Physics Department, University of California, Berkeley, California, U.S.A. (591)
- K. A. HAY, Physics Department, University of Keele, Staffordshire, England (785)
- HARRY G. HECHT, Argonne National Laboratory, Lemont, Illinois, U.S.A. (880)
- P. HELLER, Gordon McKay Laboratory, Harvard University, Cambridge, Massachusetts, U.S.A. (596)
- P. HELLER², Gordon McKay Laboratory, Harvard University, Cambridge, Massachusetts, U.S.A. (596)
- JACQUES HERVE, Université de Paris, Institut d'Electronique, Centre d'Orsay (S. et O.) France (689)
- A. HONIG, Syracuse University, Syracuse, New York, U.S.A. (439)
- J. P. IMBAUD, Laboratoire de Radioélectricité, Faculté des Sciences, Clermont-Ferrand, France (520)
- D. J. E. INGRAM, University of Keele, Staffordshire, England (809)
- C. D. JEFFRIES, University of California, Berkeley, California, U.S.A. (405)
- M. N. JONES, Department of Physics, The University of Hull, Hull, England (755)
- G. R. KHUTISHVILI, Institute of Physics of the Academy of Sciences of the Georgian S.S.S.R., Tbilisi, U.S.S.R. (486, 602)
- A. KIEL, Radiation Laboratory, The Johns Hopkins University, U.S.A. (525)
- D. KIVELSON, Department of Chemistry, University of California, Los Angeles 24, California, U.S.A. (496)
- M. P. KLEIN³, Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A. (696)
- KEI-ICHI KOGA, Institute for Solid State Physics, University of Tokyo, Azabu, Tokyo, Japan (557)
- D. C. LAINE, Physics Department, University of Keele, Staffordshire, England (785)
- H. LECAR, Columbia Radiation Laboratory, Department of Physics, Columbia University, New York, New York, U.S.A. (675)
- M. E. LINES, Clarendon Laboratory, Oxford, England (553)
- R. LONTZ, Department of Physics, Duke University, Durham, North Carolina, U.S.A. (795)
- G. W. LUDWIG, General Electric Research Laboratory, Schenectady, New York, U.S.A. (620)
- A. A. MANENKOV, P. N. Lebedev Physical Institute of the Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R. (419, 425)
- J. MARGERIE, Laboratoire de Physique de l'Ecole Normale Supérieure, Paris, France (535)
- S. A. MARSHALL, Illinois Institute of Technology, Chicago, Illinois, U.S.A. (805)
- D. MERGERIAN, Illinois Institute of Technology, Chicago, Illinois, U.S.A. (805)

¹ Present address: Department of Physics, Columbia University, New York, N.Y. U.S.A.

² Present address: Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.

³ Present address: University of California, Lawrence Radiation Laboratory, Lawrence, California, U.S.A.

- V. A. MILYAEV, P. N. Lebedev Physics Institute of the Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R. (419)
- YOSHIHITO MIYAKO, Department of Physics, Faculty of Science, Osaka University, Osaka, Japan (665)
- HIROKO MORIGAKI, Institute for Solid State Physics, University of Tokyo, Azabu, Tokyo, Japan (557, 567, 587)
- J. L. MOTCHANE, University of Besançon, Besançon, France (490)
- J. C. MURPHY, Applied Physics Laboratory, The Johns Hopkins University, Silver Spring, Maryland, U.S.A. (634)
- A. OKAYA, Columbia Radiation Laboratory, Department of Physics, Columbia University, New York, New York, U.S.A. (675, 687)
- W. OPECHOWSKI, University of British Columbia, Vancouver, Canada (463)
- R. ORBACH, Division of Engineering and Applied Physics, Harvard University, Cambridge, Massachusetts, U.S.A. (456)
- J. OWEN, Clarendon Laboratory, Oxford, England (553)
- M. B. PALMA-VITTORELLI, Istituto di Fisica dell'Università, Palermo, Italy, and Sezione Siciliana dell'Istituto Nazionale di Fisica Nucleare (582, 790)
- M. U. PALMA, Istituto di Fisica dell'Università, Palermo, Italy, and Sezione Siciliana dell'Istituto Nazionale di Fisica Nucleare (582, 790)
- F. PERSICO, Istituto di Fisica dell'Università, Palermo, Italy, and Sezione Siciliana dell'Istituto Nazionale di Fisica Nucleare (582)
- P. S. PERSHAN, Division of Engineering and Applied Physics, Harvard University, Cambridge, Massachusetts, U.S.A. (656)
- A. M. PROKHOROV, Institute of Nuclear Physics, Moscow State University, Moscow, U.S.S.R. (425)
- E. B. ROYCE, Harvard University, Cambridge, Massachusetts, U.S.A. (607)
- R. H. RUBY, University of California, Berkeley, California, U.S.A. (414)
- L. W. RUPP, JR., Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A. (836)
- P. L. SCOTT, Clarendon Laboratory, Oxford, England (399)
- G. SEIDEL, Harvard University, Cambridge, Massachusetts, U.S.A. (430, 468)
- P. E. SEIDEN, International Business Machines Corporation, Thomas J. Watson Research Center, Yorktown Heights, New York, U.S.A. (443)
- N. S. SHIREN, International Business Machines Corporation, Thomas J. Watson Research Center, Yorktown Heights, New York, U.S.A. (482)
- J. R. SINGER, University of California, Berkeley, California, U.S.A. (577)
- G. J. SLOAN, Central Research Department, E. I. du Pont de Nemours and Company, Wilmington 98, Delaware, U.S.A. (896)
- M. J. SMITH, Physics Department, University of Keele, Staffordshire, England (785)
- E. SONDER, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. (869)
- L. STALS, Interuniversity Institute for Nuclear Sciences, The Catholic University of Leuven, Leuven, Belgium (684)
- M. W. P. STRANDBERG¹, University of Grenoble, France (495)
- I. SVARE, Harvard University, Cambridge, Massachusetts, U.S.A. (430, 468)
- J. G. THEOBALD, University of Besançon, Besançon, France (490)
- J. UEBERSFELD, University of Besançon, Besançon, France (490)
- L. VAN GERVEN, Instituut voor Lage Temperaturen en Technische Fysica, The Catholic University of Leuven, Leuven, Belgium (684, 905)

¹ Present address: Massachusetts Institute of Technology, Research Laboratory of Electronics, Cambridge 39, Massachusetts, U.S.A.

- T. VÄNNGÅRD, Institute of Physics, University of Uppsala, Uppsala, Sweden (509)
- A. VAN ITTERBEEK, Interuniversity Institute for Nuclear Sciences, The Catholic University of Leuven, Leuven, Belgium (684, 905)
- W. M. WALSH, JR., Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A. (836)
- R. K. WARING, Central Research Department, E. I. du Pont de Nemours and Company, Wilmington 98, Delaware, U.S.A. (896)
- R. A. WEEKS, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. (869)
- M. WEGER, University of California, San Diego, La Jolla, California, U.S.A. (628)
- J. A. WEIL, Argonne National Laboratory, Lemont, Illinois, U.S.A. (880)
- B. J. WYLYDA, Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A. (836)
- Y. YAFET, Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A. (739)
- HENRY ZELDES, Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. (764)

P R E F A C E

7/5 - 2 - R. P.

This volume contains a collection of papers of the First International Conference on Paramagnetic Resonance held at the Hebrew University of Jerusalem, Israel on July 16-20, 1962. The conference was sponsored by the Hebrew University of Jerusalem, Israel, the International Union of Pure and Applied Physics, and the Israel Academy of Sciences and Humanities.

This conference summarized the advances which have taken place during the last 16 years since the discovery of electron spin resonance by Zavoisky. It also indicated the areas of major interests in this particular field. The topics in this conference were restricted essentially to solids. The major sections of these papers dealt with the electron spin resonance in the iron group and the rare earth groups, the theory related to these spectra, the effects of electric fields, pressure and temperature on these spectra. It discussed the advances in our knowledge of the relaxation phenomena which seem to be now reasonably well understood. Review papers on electron spin resonance in semi-conductors and in biological materials summarizes the results of the last few years in this field. Finally, there were a few selected papers on spin resonance of F centers, organic materials and in glasses.

About 180 scientists from 16 countries participated in this conference. The organizing committee wishes to express its gratitude to all the institutions which have generously assisted in making this conference possible. In addition to the three sponsoring bodies, valuable assistance has been extended by the Charles F. Kettering Foundation, the Office of Naval Research and the Israel National Council for Research and Development. We are also indebted to the National Science Foundation, the Royal Society and other national organizations for the travel support given to many of the scientists.

It is a pleasure to acknowledge the efforts of the Local Arrangements Committee, the Department of Physics of the Hebrew University, and in particular of Mrs. H. Lehrer in planning and running a smoothly conducted conference and in providing an interesting series of social events.

W. Low

Jerusalem, December, 1962

בעיה עיה-ק. ירושלים, תשכ"ג

VOLUME II — CONTENTS

PART IV: PARAMAGNETIC RELAXATION, LINE WIDTH AND EXCHANGE PHENOMENA. A.

	Page
P. L. SCOTT: Spin-Lattice Relaxation in Some Rare Earth Salts	399
C. D. JEFFRIES: Observation of the Phonon Bottleneck	405
H. BENOIT AND R. H. RUBY: An Electron Paramagnetic Resonance Spectrometer Operating between 0.3°K and 1.5°K.	414
A. A. MANENKOV AND V. A. MILYAEV: Investigation of Spin-Lattice Relaxation of S-state Ions	419
A. A. MANENKOV AND A. M. PROKHOROV: On the Temperature Dependence of Spin-Lattice Relaxation Times in Crystals	425
I. SVARE AND G. SEIDEL: Spin-Lattice Relaxation of Paramagnetic Ions in Diamagnetic Garnets	430
ARNOLD HONIG: Paramagnetic Relaxation in Small Particles	439
P. E. SEIDEN: The Determination of the Spin-Lattice Relaxation Time of Rare Earth Ions from Ferrimagnetic Resonance Experiments	443
W. I. DOBROV AND M. E. BROWNE: Low Temperature Relaxation in Ruby from Microwave Acoustic Measurements	447
R. ORBACH: Spin-Lattice Relaxation Times for Exchange Split Rare Earth Ion Levels	456

PART IV: PARAMAGNETIC RELAXATION, LINE WIDTH AND EXCHANGE PHENOMENA. B.

W. OPECHOWSKI: On the Temperature Dependence of the Shape of Paramagnetic Resonance Lines at Low Temperatures	463
G. SEIDEL AND I. SVARE: Temperature Dependence of Paramagnetic Resonance Lines	468
N. S. SHIREN: Dipolar Broadening from Pulse Velocity in Ultrasonic Spin Resonance	482
G. R. KHUTSISHVILI: Spin Diffusion and Polarization of Nuclei at Forbidden Paramagnetic Resonance	486
J. L. MOTCHANE, J. G. THEOBALD AND J. UEBERFFELD: Study of the Structure of Electron Spin Resonance Lines	490
M. W. P. STRANDBERG: Effect of Electrostatic Interactions on Dipolar Hyperfine Structure in NMR with Strong Correlation-Time Narrowing	495

	Page
DANIEL KIVELSON AND GEORGE COLLINS: ESR Line Widths in Liquids	496
J. EISINGER: Proton Relaxation Measurements as a Means of Studying Ion Binding and Certain Biological Systems	501
TÖRE VÄNNGÅRD AND ROLAND ÅASA: ESR Line Shapes of Polycrystalline Samples of $S' = 1/2$ Transition Element Ions	509
R. BATTUT, G. BERTHET, J. GRENIER AND J. P. IMBAUD: Application of the Inverted Overhauser Effect to the Detection of Free Radicals	520
A. KIEL: Line Broadening in the Excited State of Paramagnetic Crystals	525
JEAN BROSSEL AND JEAN MARGERIE: Fine Structure in the Green Absorption Band of Pink Ruby as Observed by Magnetic Resonance Technique	535

PART IV: PARAMAGNETIC RELAXATION, LINE WIDTH AND EXCHANGE PHENOMENA

C. EXCHANGE PHENOMENA

E. A. HARRIS, M. E. LINES AND J. OWEN: Paramagnetic Resonance from Three Exchange Coupled Ions	553
HIDETARO ABE, HIROKO MORIGAKI AND KEI-ICHI KOGA: Structures in Low Temperature Paramagnetic Resonance Line of Copper Potassium Chloride	557
H. ABE AND H. MORIGAKI: Paramagnetic Resonance Study in Manganese Acetate Tetrahydrate	567
J. R. SINGER: Exchange Narrowed ESR Absorption Lines at Low and Intermediate Frequencies	577
T. GAROFANO, M. B. PALMA-VITTORELLI, M. U. PALMA AND F. PERSICO: Motional and Exchange Effects in the ESR Behaviour of Ni^{2+} and Mn^{2+} Hexamine Cubic Crystals	582
H. ABE AND H. MORIGAKI: Temperature Dependence of Line Width in Copper Trichloroacetate Monohydrate	587
A. G. ANDERSON AND S. R. HARTMANN: Nuclear Magnetic Spectra and Relaxation in the Demagnetized State	591
P. HELLER AND G. B. BENEDEK: Magnetic Resonance Determination of the Susceptibility in Antiferromagnetic MnF_2	597
G. R. KHUTISHVILI: On Influence of Saturation of Cyclotron Resonance in Degenerated Zone on Nuclear Resonance	602

PART V: EFFECTS OF ELECTRIC FIELD, EXTERNAL PRESSURE ON ESR SPECTRA AND EXPERIMENTAL TECHNIQUES

A. Effects of Electric Field and External Pressure on ESR

N. BLOEMBERGEN AND E. B. ROYCE: Electric Shift of the Cr^{3+} Magnetic Resonance in Ruby	607
--	-----

	Page
G. W. LUDWIG AND F. S. HAM: Electric Field Effects in Paramagnetic Resonance	620
M. WEGER AND ELSA FEHER: The Second Order Effect of Applied Electric Fields on the Electron Spin Resonance of Impurity Ions in MgO	628
J. O. ARTMAN AND J. C. MURPHY: Hemihedral Field Effects in the Spectrum of Ruby	634
P. S. PERSHAN AND N. BLOEMBERGEN: Electric Shift of the F^{19} Hyperfine Interaction in Antiferromagnetic MnF_2	656
MUNEYUKI DATE AND YOSHIHITO MIYAKO: Electron Spin Resonance of Some Magnetic Ions in TiO_2 Under an External Stress	665

PART V: EFFECTS OF ELECTRIC FIELD, EXTERNAL PRESSURE ON ESR SPECTRA AND EXPERIMENTAL TECHNIQUES

B. Experimental Techniques

H. LECAR AND A. OKAYA: A Maser Paramagnetic Resonance Spectrometer	675
L. VAN GERVEN, A. VAN ITTERBEEK AND L. STALS: A Phase-Selective X-Y-Recorder for Magnetic Resonance Experiments	684
A. OKAYA: EPR Spectra of OH, Ti^{3+} Ions and Color Centers in Rutile as Revealed by a High Sensitivity Dielectric Resonance Spectrometer	687
JACQUES HERVE: Measurement of Electronic Spin-Lattice Relaxation Times by Rapid Modulation of the Saturation Factor	689
M. P. KLEIN AND G. W. BARTON: Enhancement of Signal-to-Noise Ratio by Continuous Averaging	698
HARMON W. BROWN: The Application of Molecular Orbital Theory to Spectroscopic Splitting Factors	704

PART VI: ESR OF SEMICONDUCTORS, F CENTERS AND PHOSPHORUS AND RADIATION DAMAGE

G. FEHER: Review of Electron Spin Resonance Experiments in Semiconductors	715
Y. YAFET: g -Factors and Spin-Lattice Relaxation of Conduction Electrons	739
T. E. FEUCHTWANG: The Electron Nuclear Double Resonance Spectrum of an F -Center in Alkali Halides	740
T. E. FEUCHTWANG: The Electric Field Gradient Seen by Nuclei in the First Few Shells about the Vacancy Associated with an F -center in Alkali Halides	749
A. CUNLIFFE, G. F. J. GARLICK AND M. N. JONES: The Correlation of the Electron Spin Resonance Spectra and the Luminescence Properties of Some Manganese Activated Phosphors	755
HENRY ZELDES: Paramagnetic Species in Irradiated KNO_3	764

	Page
M. J. A. SMITH, K. A. HAY AND D. C. LAINE: Electron Resonance Investigations of U. V. Irradiated Hydrides and Bromides	785
L. BELLOMONTE, M. B. PALMA-VITTORELLI AND M. U. PALMA: Trapping of Photo-produced Holes in Cu ⁺ -Doped AgCl Crystals	790
R. LONTZ AND W. GORDY: Fluorine Hyperfine Interaction in the ESR of Irradiated Organic Single Crystals	795
D. MERGERIAN AND S. A. MARSHALL: Irradiation Produced Paramagnetic Oxides of Nitrogen in Single Crystal Potassium Azide	805

PART VII: ESR OF BIOLOGICAL MATERIALS, ORGANIC CRYSTALS AND GLASSES

D. J. E. INGRAM: Paramagnetic Resonance in Biological Materials	809
W. M. WALSH JR., L. W. RUPP JR. AND B. J. WYLUDA: Paramagnetic Resonance Studies of Magnetic Ions Bound in Nucleic Acid Pseudocrystals	836
S. E. HARRISON AND J. M. ASSOUR: Electron Spin Resonance of Copper Phthalocyanine	855
R. A. WEEKS AND E. SONDER: The Relation Between the Magnetic Susceptibility, Electron Spin Resonance, and the Optical Absorption of the E'_1 Center in Fused Silica	869
J. A. WEIL, G. L. GOODMAN AND H. G. HECHT: Paramagnetic Resonance Absorption in Peroxo Dicobalt Complexes — Single Crystal Studies	880
R. K. WARING JR. AND G. J. SLOAN: Trapping in Solution of Non-Equilibrium Concentrations of Biradicals	896
L. VAN GERVEN, A. VAN ITTERBEEK AND L. DE LAET: Low Field EPR Measurements in DPPH at Low Temperatures	905

VOLUME I — CONTENTS

Page

PART I: ESR SPECTRA OF IRON GROUP ELEMENTS. A.

H. J. GERRITSEN: Paramagnetic Resonance of Transition Metal Ions in Rutile (TiO_2)	3
G. M. ZVEREV AND A. M. PROKHOROV: Electron Spin Resonance of Rutile with Cobalt	13
K. A. MÜLLER: Paramagnetic Resonance and Optical Absorption of Transition Element Ions in SrTiO_3 and LaAlO_3	17
D. KIRO, W. LOW AND A. ZUSMAN: ESR Spectra of Cr^{3+} and Gd^{3+} in Lanthanum Aluminate	44
L. RIMAI AND G. A. DEMARS: Electron Paramagnetic Resonance of Some Rare Earth Impurities in Strontium Titanate	51
R. S. RUBINS AND W. LOW: On the Paramagnetic Resonance Spectra of Some Rare Earth and Iron Group Impurities in Strontium Titanate	59
V. J. FOLEN: Paramagnetic Resonance of Fe^{3+} in Spinel-type Single Crystals	68

PART I: ESR SPECTRA OF IRON GROUP ELEMENTS. B.

W. LOW AND R. S. RUBINS: Paramagnetic Resonance of Iron Group and Rare Earth Impurities in Calcium Oxide	79
P. AUZINS, J. W. ORTON AND J. E. WERTZ: Electron Spin Resonance Studies of Impurities in II-VI Compounds	90
J. S. VAN WIERINGEN AND J. G. RENSEN: Influence of Lattice Imperfections on the Paramagnetic Resonance of V^{2+} and Cr^{3+} in MgO	105
S. GESCHWIND, P. KISLIUK, M. P. KLEIN, J. P. REMEIKI AND D. L. WOOD: Sharp Line Fluorescence, EPR and Thermoluminescence of Mn^{4+} in $\alpha\text{-Al}_2\text{O}_3$	113
W. E. BLUMBERG, J. EISINGER, S. GESCHWIND AND J. P. REMEIKI: Paramagnetic and Endor Spectrum of Cu^{3+} in Al_2O_3	125
L. S. KORNIENKO AND A. M. PROKHOROV: Electron Spin Resonance and Spin-Lattice Relaxation of Ti^{3+} Ion in Corundum	126
F. S. HAM AND G. W. LUDWIG: Paramagnetic Properties of Iron Group Ions in Tetrahedral Coordination	130
T. L. ESTLE, G. K. WALTERS AND M. DEWIT: Paramagnetic Resonance of Cr in CdS	144
A. BOSE, R. CHATTERJEE AND A. S. CHAKRABORTY: Optical and Magnetic Behaviors of $\text{Ni}^{2+} \cdot 6\text{H}_2\text{O}$ Complex in Crystalline Salts	155

PART II: ESR SPECTRA OF RARE EARTH AND URANIUM ELEMENTS

A. Experimental Results of ESR Spectra of $4f^n$ and $5f^n$ Ions

	Page
W. HAYES AND J. W. TWIDELL: Paramagnetic Resonance of Irradiated CaF_2 Containing Rare Earth Salts	163
W. LOW AND U. RANON: ESR of Rare Earth Ions in Irradiated and Thermally Treated CaF_2	167
REUBEN S. TITLE: Paramagnetic Resonance of U^{3+} and U^{4+} in Calcium and Strontium Fluoride	178
A. YARIV: Paramagnetic Resonance and Charge Compensation of Tetravalent Uranium (U^{4+}) in Calcium, Strontium, and Barium Fluorides	189
P. P. PASHININ AND A. M. PROKHOROV: Electron Spin Resonance and Spin-Lattice Relaxation for the Yb^{3+} Ion in CdF_2	197
J. M. BAKER, J. P. HURRELL AND F. I. B. WILLIAMS: Electron Nuclear Double Resonance in Calcium Fluoride Containing Divalent Europium	202
J. L. HALL AND T. R. SCHUMACHER: Electron Spin Resonance of Interstitial Hydrogen Atoms in CaF_2	206
H. A. BUCKMASTER: Angular Spectra of $\Delta M = \pm 2$ and ± 3 Transitions in $(0.999 \text{ La}, 0.001 \text{ Gd}) \cdot (\text{C}_2\text{H}_5\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$	217
J. OVERMEYER, E. A. GIESS, M. J. FREISER AND B. A. CALHOUN: Paramagnetic Resonance of Gd^{3+} in Garnet Crystals and Its Relation to the Anisotropy of GdIG	224

PART II: ESR SPECTRA OF RARE EARTH AND URANIUM ELEMENTS

B. Theoretical Aspects of ESR in Rare Earth Ions

G. H. DIEKE: Energy Levels of and Energy Transfer in Rare Earth Salts	237
J. C. EISENSTEIN: The Validity of Crystal Field Theory as Applied to Rare Earth Ions: An Analysis of the Spectrum of Praseodymium Trichloride	253
G. BURNS: Shielding and Crystal Fields at Rare Earth Ions	260
M. J. LEASK, R. ORBACH, M. J. D. POWELL AND W. P. WOLF: Crystalline Field Splittings in Cerium Magnesium Nitrate	261
Y. AYANT: Quelques Propriétés des Niveaux Cristallins Γ_8 en Symétrie Cubique	267
Y. AYANT ET J. THOMAS: Etude Théorique du Blocage du Moment Magnétique des Ions Terres Rares dans les Gallates à Structure Grenat	279
E. BELORIZKY ET Y. AYANT: Etude de la Structure Hyperfine de l'Ion Pr^{3+} dans le Gallate de Praséodyme	290

PART III: THEORY RELATED TO ESR

	Page
W. HAUSER: On the Spin-Hamiltonian Description of Energy Levels in Crystals	297
A. S. CHAKRAVARTY AND R. BERSOHN: Zero Field Splitting in Atomic Nitrogen	305
W. LOW AND G. ROSENGARTEN: The Ground State Splitting and Optical Spectra of d^5 Configuration in Cubic Crystalline Fields	314
M. C. M. O'BRIEN: The ESR Spectrum of a d^9 Ion in an Octahedral Environment	322
ROBERT ENGLMAN AND DAVID HORN: Anomalies of g -factor due to Vibrational Coupling	329
W. MARSHALL: Hyperfine Interactions with Ligand Nuclei in Transition Ion Complexes	347
G. F. KOSTER AND H. STATZ: Exchange Splittings of L-S Multiplets of Rare Earth Ions in Crystals	362
A. J. FREEMAN AND R. E. WATSON: A Theoretical Investigation of Some Spectroscopic and Magnetic Properties of Rare Earth Ions	373
D. F. JOHNSTON: The Direct Magnetic Contribution to the Transferred Hyperfine Interaction for Trivalent Rare Earth Ions	374
I. R. SENITZKY: Resonant Harmonic Generation by Paramagnetic Ions	380
VERNON W. HUGHES: Muon Resonance	382

PART I

ESR SPECTRA OF IRON GROUP ELEMENTS

A.

Paramagnetic Resonance of Transition Metal Ions in Rutile (TiO₂)

H. J. GERRITSEN

Chalmers University of Technology, Gothenburg, Sweden*

ABSTRACT

A review and discussion of paramagnetic resonance on eighteen different ions in TiO₂ will be given, with emphasis on charge, lattice site and crystal field considerations.

Introduction

Rutile (TiO₂) is a crystal with tetragonal symmetry. Thick crystals are slightly yellow due to the fundamental absorption of the crystal which sets in at about 4300 Å [1]. There are two lattice sites at which the Ti⁴⁺ ions are located. These sites are identical except for a 90° rotation around the tetragonal axis (see Figure 1a). The local surroundings of this site has cubic symmetry with a rather small orthorhombic distortion. The lines

Part of rutile lattice showing the two substitutional Ti⁴⁺ positions.

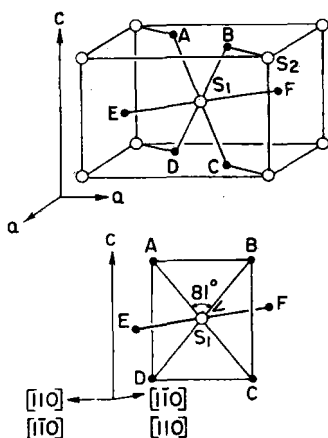


Figure 1a

SA = SB = SC = SD = 1.94 Å
SE = SF = 1.99 Å
○ = Ti⁴⁺
● = O²⁻
□ = Interstitial position

Part of rutile lattice showing the four interstitial positions.

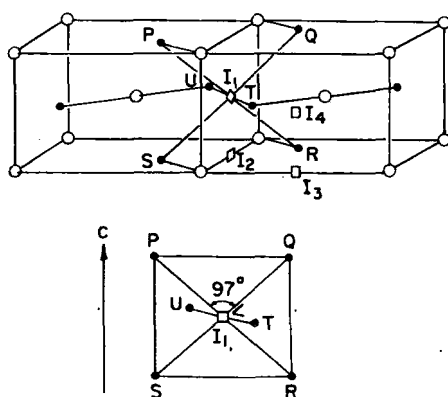


Figure 1b

IP = IQ = IR = IS = 2.23 Å
IU = IT = 1.67 Å

Substitutional and interstitial lattice positions in TiO₂.

* Present address: RCA Laboratories, Princeton, N. J.