REPORT RESUMES

ED 020 904 SE 004 901

DEVELOPMENT OF A MULTI-COORDINATE VOCABULARY, CHEMICAL PHYSICS.

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AMERICAN INST. OF PHYSICS, NEW YORK, N.Y.

PUB DATE MAR 68

EDRS PRICE MF-$0.25 HC-$1.04 24P.

DESCRIPTORS- *COLLEGE SCIENCE, *CHEMISTRY, *INFORMATION SCIENCE, *INFORMATION RETRIEVAL, *THESAURI, VOCABULARY, GRADUATE STUDY, PHYSICS, SCIENTIFIC RESEARCH, AMERICAN INSTITUTE OF PHYSICS, NATIONAL SCIENCE FOUNDATION,

THIS PAPER DESCRIBES A METHOD (SCHEME) FOR THE DEVELOPMENT OF A VOCABULARY IN THE FIELD OF CHEMICAL PHYSICS FROM PRIMARY JOURNAL ARTICLES. ALL TERMS APPEARING IN A RECENT JOURNAL (VOL. 39, JOURNAL OF CHEMICAL PHYSICS) JUDGED TO BE IMPORTANT WERE DIVIDED INTO THREE CATEGORIES--(1) PROPERTIES, PROCESSES, PHENOMENA, (2) OBJECTS, INCLUDING SYSTEMS AND MATERIALS, AND (3) METHODS, INCLUDING DEVICES. IN ADDITION TO THESE THREE CLASSIFICATIONS, TERMS SPECIFYING SPECIAL CONDITIONS WERE ALSO USED SUCH AS MASS, ENERGY, AND TEMPERATURE. BY THE THREE MAJOR CLASSIFICATIONS AND APPROPRIATE ADDITIONAL TERMS DESCRIBING CONDITIONS, A MULTI-COORDINATED INDEX IS ESTABLISHED. THE THESAURUS WAS REVIEWED BY SPECIALISTS WHO GAVE SUGGESTIONS FOR REVISIONS AND ADDITIONS. ADDITIONAL TERMS WERE ADDED IN THE PROCESS OF USING THE THESAURUS IN EXPERIMENTAL RETRIEVAL. THE COMPLETE VOCABULARY IS INCLUDED IN THE PAPER. METHODS USED TO DEVELOP THIS THESAURUS WERE ALSO USED TO DEVELOP THESAURI FOR THE FIELDS OF PLASMA PHYSICS AND LASERS AND MASERS. THE PAPERS WHICH WERE INDEXED ACCORDING TO THIS SYSTEM FORM THE DATA BASE FOR A NUMBER OF EXPERIMENTS CURRENTLY BEING CONDUCTED ON RETRIEVAL MECHANISMS. (DH)

Received in RSP 4/17/68 ID 68-3
No. of copies 7 (March 1968)
Grant (Contract) No. GN-549

DEVELOPMENT OF A MULTI-COORDINATE VOCABULARY:

CHEMICAL PHYSICS

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This program supported by the National Science Foundation under Grant No. NSF-GN-549

Development of a Multi-coordinate Vocabulary: Chemical Physics

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A number of thesauri have been created in the past by bringing together groups of subject experts to determine relevant terms, or by merging lists of terms derived from various sources within a field. This paper describes a method of creating of a vocabulary derived from primary journal articles. The method is applied to the development of a vocabulary in the field of chemical physics. The vocabulary takes the form of a set of authority lists.

The chemical physics vocabulary was created directly from a group of articles published in the largest journal in the field of chemical physics. Volume 39 of the Journal of Chemical Physics (a total of about 860 articles) was read through, and all terms appearing in the title, abstract or body of the paper which were judged to be important terms by the author were placed on cards. Taking the definition of physics to be "the study of the properties of objects by methods," it was then possible to divide the cards into the following lists or coordinates:

1. Properties, Processes and Phenomena.
2. Objects, including systems and materials.
3. Methods, including devices.

Additional terms describe whether the paper is experimental, theoretical or both, and special conditions such as mass, energy, frequency, temperature or pressure ranges. One can then classify a paper by assigning one or more descriptors from each of the three lists plus appropriate additional terms describing conditions, producing a multi-coordinate index.

The thesaurus developed in this manner contained only terms referring to articles appearing in Vol. 39 of JCP. It was then reviewed by subject specialists who gave suggestions for revisions and additions. Some additional terms were added to the thesaurus as the need for them appeared during the process of indexing papers for experiments in retrieval. The complete vocabulary appears in Appendix A.

The list of properties, processes and phenomena is organized hierarchically, with synonyms or very closely related terms (quasi-synonyms) treated as one descriptor. Papers are indexed at the most specific level possible, but can be searched for at a broader level. For example, Fluid Properties has a subheading Fluid Transport Properties, with further subdivisions into terms such as Thermal Conductivity and Viscosity; Viscosity is further subdivided into Volume Viscosity and Shear Viscosity. A particular journal article may report an experimental measurement of Shear Viscosity which may be relevant to the interests of someone working in the general field of Fluid Transport Properties or may be of interest to someone who wants the specific measurement. In a computer search, it should then be possible to ask for all papers on Viscosity or all papers on Fluid Transport Properties, including Viscosity; in our system it is possible to cover a range of related terms in a computer search merely by specifying the first and last terms to be included in the search. For convenience in handling the indexed papers within the computer, all of our index terms were converted to 7-digit code numbers, which indicate the coordinate of the term (property, object or method) as well as the term's level in the hierarchy. An internal dictionary converts the code numbers back to English language for the printed output.

The list of objects is a faceted list. The facets consist of the following:

1. An identification of the physical nature of the object, e.g., electron, atom, molecule, etc., together with a nonunique notation of the chemical formula.

2. The physical class of the object, i.e., semiconductor, polymer, etc.
3. The physical state of the object, i.e., single crystal, monolayer film, etc.
4. Systems, such as rigid rotors or spin systems.
5. Shape of the object, used primarily for theoretical papers in chemical physics in which a shape must be assumed in order to perform calculations on a particular model of the object.

One object has several facets. If the paper deals, however, with the properties of several objects, the article may be treated as if it were a series of papers, each object being indexed by the appropriate set of properties.

The list of methods describes experimental and theoretical methods, and some of the devices used to make measurements. The revised thesaurus was used to index some 4,000 articles from the Journal of Chemical Physics volumes 41-44 July, 1964 - June, 1966. Examples of indexed papers appear in Appendix B.

The method used to develop this thesaurus was also used to develop thesauri for the fields of plasma physics and lasers and masers.

The approximately 850 papers appearing in volume 44 of the Journal of Chemical Physics which were indexed according to this method form the data base for several experiments now being conducted on retrieval mechanisms. One of these is a joint experiment with the Chemical Abstracts Service to determine the needs of chemical physicists and physical chemists, and the types of indexing necessary to meet these needs. Another experiment with this data base will produce a printed index permuted on the property and methods lists. The results of these experiments will be discussed in later reports.

Acknowledgment

The author gratefully acknowledges helpful discussions with the following, during the development of the chemical physics vocabulary:

Prof. Benjamin P. Dailey	Columbia University
Prof. George K. Fraenkel	Columbia University
Prof. Martin Goldstein	Yeshiva University
Prof. Martin Karplus	Harvard University
Prof. Daniel Kivelson	U.C.L.A.
Prof. Jeremy Musher	Yeshiva University
Prof. Irwin Oppenheim	M.I.T.
Prof. William Spindel	Yeshiva University

APPENDIX A
CHEMICAL PHYSICS VOCABULARY

PROPERTIES, PROCESSES AND PHENOMENA

- Acoustics and Ultrasonics
    - Sound Velocity
    - Ultrasonic Attenuation

- Bond Structure
    - Bond Hybridization
    - Bond Resonance Integral
    - Covalence and Ionic Character
    - Conjugation and Hyperconjugation
    - Electronegativity
    - Hydrogen Bonding

- Charge Distribution (see also Electron Properties)
    - Charge Transfer
        - Charge-transfer cross-section
        - Charge-transfer energy
    - Multipole Interaction
        - Dipole-Dipole Interaction
        - Dipole-Quadrupole Interaction
        - Dipole-Induced Dipole Interaction
        - Induced Dipole-Induced Dipole Interaction
        - Quadrupole-Quadrupole Interaction
    - Electric Field Gradient
    - Electronic Structure
    - Induced Dipole
    - Polarizability
    - Nuclear Quadrupole Resonance
        - Spectra
            - Frequency
            - Intensity
            - Line Shape
            - Line Width
    - Quadrupole
        - Asymmetry Parameter
        - Quadrupole Moment
        - Quadrupole Coupling Constant

- Chemical Properties
    - Catalysis
        - Catalysis, Temperature Dependence
        - Heterogeneous Catalysis
        - Homogeneous Catalysis
    - Kinetics of Reaction
        - Activation Energy
        - Equilibria
        - Rates of Reaction
        - Reaction Cross-section; Reaction Probability
        - Reaction Mechanism
    - Reduction and Oxidation

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

- Collision Processes and Scattering (see also Energy Transfer)
    - Angular Distributions and Trajectories
    - Collisions
        - Capture Cross-sections
        - Collision Cross-sections; Collision Diameters; Collision Efficiency
        - Elastic Collisions
        - Inelastic Collisions

- Scattering
    - Energy-Dependent Scattering
    - Energy-Independent Scattering
    - Energy-Loss Parameter; Energy Loss Spectra
    - Energy-transfer Cross-section
    - Scattering Cross-section

- Colloidal Properties
    - Stability
    - Micelle Formation
    - Micelle Structure

- Detonation and Shock Waves
    - Activation Energy
    - Mechanism of Initiation
    - Induction Time

- Electric and Dielectric Properties
    - Conductivity
    - Dielectric Constant
    - Dielectric Loss
    - Dielectric Relaxation Time
    - Hysteresis
    - Dielectric Strength
    - Ionic Mobility
    - Transport Number
    - Electrical Resistance

- Electron Properties
    - Electron Charge Density
    - Electron Spin Density
    - Electron Transfer
    - Rotation-Electron Spin Interaction
    - Spin-Orbit Interaction

- Electronic States
    - Electronic Spectra
        - Absorption Cross-section; Absorption Coefficient
        - Band Width
        - Frequency
        - Intensity
        - Lifetime
        - Stark Effect, Electronic Spectra
    - Term Values
    - Transition Probability
    - Electronic Energy Transfer
    - Vibronic Coupling

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

- Energy Transfer (see also Collision Processes and Scattering; Luminescence)
  - Electronic Energy Transfer
  - Energy Transfer between rotation and vibrational degrees of freedom
  - Energy Transfer Cross-section
  - Energy Transfer Mechanism
  - Radiationless Transition
  - Thermal Energy Transfer
  - Energy Transfer Probability; Transition Probability
  - Energy Transfer, Translational-Vibrational
  - Energy Transfer, Electronic-Vibrational

- Energy and Potentials (see also Wave Functions, Eigenfunctions and Integrals)
  - Binding Energy; Dissociation Energy
  - Charge Transfer Energy
  - Electron-Electron Repulsion Energy
  - Electron-Nuclear Attraction Energy
  - Energy Derivatives
  - Energy Level
  - Energy Level Density
  - Excitation Energy
  - Ground State Energy
  - Hartree-Fock Energy
  - Interaction Potential
  - Ionization Energy; Electron Affinity
  - Lattice Energy
  - Kinetic Energy
  - Orbital Energy
  - Pi-electron Energy
  - Potential Energy; Potential Energy Surface; Barrier Heights and Widths
  - Potential Function; Potential Constants
  - Predissociation
  - Relativistic Energy
  - Resonance Energy
  - Rotational Energy
  - Sigma-electron Energy
  - Strain Energy
  - Total Energy
  - Translational Energy
  - Tunneling
  - Vibrational Energy
    - Torsional Energy

- Fluid Properties (see also Solutions; Thermodynamic Properties; Transport Properties
  - Critical Properties
    - Critical Opalescence
  - Dielectric Relaxation Time
  - Equation of State
    - Virial Coefficients
    - Volume
    - Pressure
  - Flow Birefringence
  - Interaction Properties; Intermolecular Interaction

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

- Intramolecular Interaction
- Pair Potential
- Distribution Function; Correlation Function
- Scattering Potential
- Fluid Structure; Structural Domains
- Structural Relaxation Time
- Surface Tension
- Transport Properties
    - Diffusion and Self-Diffusion Coefficients
    - Thermal Diffusion Coefficient
    - Electrical Conductivity
    - Density
    - Ionic Mobility
    - Sedimentation
    - Viscosity
        - Volume Viscosity
        - Shear Viscosity
    - Thermal Conductivity
    - Viscoelastic Properties
    - Transport Numbers
- Triplet Distribution
- Cluster Integrals
- Effusion

Ionic Properties (see also Photoionization)

- Auto-ionization
- Donnan Equilibrium Parameter
- Ionic Mobility
- Ion Exchange
    - Distribution Coefficients
    - Thickness of effective boundary layers
- Kinetic Energy
- Ion Mass
- Ion Formation
- Ionic Vibrational Levels
- Ionization Potential; Ionization Energy
- Ionization Processes
- Ionization Cross-section; Ion Yields
- Field Ionization

Isotope Effects (see also Nuclide Properties)

- Equilibrium Isotope Effects
- Intermolecular Isotope Effects
- Intramolecular Isotope Effects
- Isotope Separation; Isotope Separation Factor
- Kinetic Isotope Effects

Laser and Maser Properties

Liquid Crystal Properties

- Domains
- Electric and Magnetic Field Effects
- Optical Properties

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

- Luminescence (see also Energy Transfer)
    - Spectra
        - Intensities
        - Lifetime; Quenching; Quenching Cross-section
        - Yield
    - Chemiluminescence
    - Thermoluminescence

- Macromolecular Properties (see also Kinetics of Reaction; Thermodynamic Properties; Transport Properties)
    - Donnan Equilibrium Parameter
    - Molecular Shape
    - Molecular Size
    - Molecular Weight Distribution
    - Polymer Formation
    - Polymer Length
    - Hydrodynamic Interaction Parameter

- Magnetic Properties
    - Anisotropy, Magnetic
    - Antiferromagnetism
        - Neel Temperature
    - Curie Temperature
    - Electron Paramagnetic Resonance
        - Correlation Time
        - Gyromagnetic Ratio
        - Hyperfine Interactions
        - Relaxation Time
        - Spectra
            - Frequency
            - Line Shape
            - Line Width
            - Intensity
            - Double Quantum Transitions
        - Superhyperfine Interactions
        - Zero-field Splitting
        - Spin-Spin Coupling
    - Magnetic Coupling Constant
    - Magnetization
    - Magnetic Entropy
    - Magnetic Moment
        - Rotational Magnetic Moment
    - Magnetic Susceptibility
    - Nuclear Magnetic Resonance
        - Spectra
            - First Moments
            - Second Moments
            - Double Quantum Transitions
            - Chemical Shift
            - Double Resonance
            - Line Shape
            - Line Width

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

        - Nuclear Spin-Spin Coupling
        - Nuclear Spin-Rotation Interaction
        - Nuclear Shielding Constants
        - Nuclear Spin Relaxation Time
    - Ferromagnetism
    - Overhauser Effect

- Mass Spectra
    - Ionization and Appearance Potentials
    - Ionization Probability
    - Partial Ionization Cross-section

- Mossbauer Spectra

- Molecular Structure
    - Bond Distances and Bond Angles
    - Isomerism
    - Molecular Shape
    - Molecular Size
    - Steric Effects
    - Moment of Inertia; Rotational Constants

- Nuclear Properties (see also Nuclear Magnetic Resonance; Nuclear Quadrupole Resonance)
    - Nuclear Shielding Constants
    - Spin Conversion, ortho-para
    - Nuclear Spin Relaxation Time

- Nuclide Properties
    - Abundance
    - Mass
    - Spin

- Optical Properties
    - Anisotropy, Optical
    - Birefringence
    - Dichroism
    - Diffraction
    - Gouy Fringes
    - Optical Rotation
    - Photon Effects
        - Lifetime
        - Photoconduction
            - Activation Energy
            - Quantum Yield, Photoconduction
        - Photoelectric Effect (includes photosensitivity)
        - Photoemission
        - Photochemical Decomposition and Formation
            - Quantum Yield, Photochemistry
        - Photoionization
        - Multi-Photon Processes
    - Pleochroism

- Reflectance; Reflectivity
- Refraction
  - Index of Refraction; Refractive Index
- Scattering Properties, Optical; Transmission Coefficients, Optical

Quantum Mechanical Properties

Hamiltonians
- Spin Hamiltonian

Symmetry Properties
- Parity
- Time Reversal

Wave Functions and Eigenfunctions
- Eigenfunctions
- Orbital Angular Momentum Wave Functions
- Orthogonalized Orbitals
- Spin Eigenfunctions

Wave Function Integrals and Matrix Elements
- Expectation Values
- Overlap Integrals
- Transition Probabilities
- Bond Resonance Integrals
- One-electron, One-center Integrals
- One-electron, Two-center Integrals
- Three-center and Four-center Integrals

Radiation Effects
- Conductance
- Ion Formation
- Ion Yield
- Ionization
- Ionization Energy
- Ionization Probability; Ionization Cross-Section
- Radiation Products
  - Stability of Radiation Products
- Temperature Dependence, Radiation Effects

Radiochemistry
- Spontaneous Transmutation, Beta-Decay
- Radiative Neutron Capture
- Decay Schemes
- Isomeric Transitions
- Positronium Lifetime

Relaxation Time and Relaxation
- Dissociation Relaxation Time
- Electron Spin Resonance Relaxation Time
- Dielectric Relaxation Time
- Ionization Relaxation Time

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

  - Nuclear Spin Relaxation Time
  - Relaxation Time Spectra
  - Rotational Relaxation Time
  - Structural Relaxation Time
  - Vibrational Relaxation Time
  - Thermal Relaxation Time
  - Quadrupole-Coupled Relaxation
  - Magnetic Dipole Spin-Spin Relaxation

- Rotation
  - Coriolis Effects
  - Internal Rotation
  - Molecular Rotation
  - Rotational Spectra
    - Frequency
    - Line Shape
    - Line Width
    - Rotational Constants; Moment of Inertia
    - Selection Rules
    - Stark Effect
    - Zeeman Effect
    - Lambda Doubling
    - Intensity
  - Nuclear Spin-Rotation Interaction
  - Rotation-Electron Spin Interaction
  - Rotation-Vibration Interaction
  - Rotational Relaxation Time
  - Rotational-Vibronic Interaction

- Solid State Properties
  - Crystal Structure and Crystal Dynamics
    - Atom Position
    - Cation Distribution
    - Defects
    - Lattice Energy
    - Lattice Parameters
    - Lattice Vibrations
    - Microstructure
    - Crystal Surfaces
      - Surface Distortion
      - Surface Energy
    - Unit Cell
  - Crystal Growth
    - Rate of Nucleation
  - Crystal Spectra
    - Crystalline Field Parameters
    - Electric and Magnetic Dipole Transitions
    - Irreducible Representations
    - Intensity
    - Frequency
    - Stark Effect
    - Temperature Dependence of Spectra
    - Zeeman Effect

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

- Optical Properties of Solids (see also Optical Properties)
  - Color Centers
  - Photoemission
  - Photoeffects
  - Reflectivity
- Electric and Magnetic Properties of Solids
  - Carrier Mobility
  - Ionic Conductivity
  - Electron Mobility
  - Holes
  - Ionic Diffusion
  - Photoconductivity
  - Piezoelectricity
  - Polarizability
  - Transition from Semiconductor to Metallic State
- Thermoelectric Effects
  - Seebeck Coefficients
  - Trap Depths
- Transport Properties
  - Electrical Conductivity
  - Thermal Conductivity
  - Thermal Diffusion Coefficient
  - Diffusion
  - Viscoelastic Properties

Solutions (see also Fluid Properties)
- Donnan Equilibrium Parameter
- Reaction Mechanisms
- Structure of Solutions
- Solvent Effects
- Ionic Mobility
- Critical Properties

Spin Properties
- Electron Spin-Rotation Interaction
- Electron Spin-Spin Coupling
- Nuclear Spin-Spin Coupling
- Spin Conversion, ortho-para
- Nuclear Spin-Rotation Interaction
- Spin Hamiltonian
- Spin-Orbit Coupling
- Spin Susceptibility
- Electron Spin Relaxation Time
- Nuclear Spin Relaxation Time

Surface and Film Properties (see also Solid State Properties)
- Accommodation Coefficients
- Sorption
  - Absorption
  - Adsorption
  - Chemisorption
  - Desorption
- Film Thickness
- Surface Tension

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

- Thermodynamic Properties and Thermal Properties
  - Accommodation Coefficients
  - Activity
  - Compressibility
  - Critical Properties
    - Critical Point
  - Density
  - Energy
    - Configurational Energy
    - Energy of Activation
    - Energy of Formation and Dissociation
    - Energy of Fusion
    - Energy of Hydration
    - Energy of Mixing
      - Energy of Solution
    - Energy of Transition
    - Energy of Vaporization
      - Energy of Evaporation
      - Energy of Sublimation
    - Zero-point Energy
  - Enthalpy
    - Enthalpy of Activation
    - Enthalpy of Formation and Dissociation
    - Enthalpy of Fusion
    - Enthalpy of Hydration
    - Enthalpy of Mixing
      - Enthalpy of Solution
    - Enthalpy of Transition
    - Enthalpy of Vaporization
      - Enthalpy of Evaporation
      - Enthalpy of Sublimation
  - Entropy
    - Entropy of Activation
    - Entropy of Formation and Dissociation
    - Entropy of Fusion
    - Entropy of Hydration
    - Entropy of Mixing
      - Entropy of Solution
    - Entropy of Transition
    - Entropy of Vaporization
      - Entropy of Evaporation
      - Entropy of Sublimation
  - Equation of State
    - Virial Coefficients
  - Formation Constant; Association Constant
  - Free Energy
    - Free Energy of Activation
    - Free Energy of Formation and Dissociation
    - Free Energy of Fusion
    - Free Energy of Hydration
    - Free Energy of Mixing
      - Free Energy of Solution

PROPERTIES, PROCESSES AND PHENOMENA (CONT.)

-
    -
        - Free Energy of Transition
        - Free Energy of Vaporization
            - Free Energy of Evaporation
            - Free Energy of Sublimation
    - Heat Capacity
    - Partition Functions
    - Phase Transition
    - Phase Diagram
    - Pressure
        - Partial Pressure
        - Vapor Pressure
    - Temperature
    - Thermal Conductivity
    - Thermal Diffusion
    - Thermal Expansion Coefficient
    - Volume
        - Free Volume
        - Partial Molar Volume
    - Work Function

- Vibrational Properties
    - Rotation-Vibration Interaction
    - Vibrational Energy
    - Vibrational Coupling
    - Vibrational Spectra
        - Anharmonicity
        - Force Constants
        - Infrared Spectra
            - Intensities
        - Raman Spectra
        - Intermolecular Coupling
        - Potential Function; Potential Constants
        - Selection Rules, Symmetry Classifications and Irreducible Representations
        - Torsional Oscillations
        - Pressure Effects
        - Line Shape
        - Normal Coordinates
        - Fundamental Modes

- X-ray Spectra

APPENDIX A
CHEMICAL PHYSICS VOCABULARY

METHODS

- Acoustics and Ultrasonics
- Atomic and Molecular Spectroscopy
  - Mass Spectroscopy
    - Time-of-flight mass spectrometer
  - Mossbauer Spectroscopy
  - Neutron Diffraction
  - X-Ray Diffraction
  - Emission Spectroscopy
  - Ultraviolet and Visible Spectroscopy
  - Infrared and Near Infrared Spectroscopy
  - Raman Spectroscopy
  - Far Infrared Spectroscopy
  - Microwave Spectroscopy
    - Beam-maser Microwave Spectroscopy
  - Non-resonant Microwave Spectroscopy
  - Electron Paramagnetic Resonance
  - Nuclear Magnetic Resonance
  - Nuclear Quadrupole Resonance
  - X-Ray Spectroscopy

- Beams
  - Atomic Beams
  - Electron Beams
  - Molecular Beams

- Chemical Processes
  - Chemical Analysis
  - Chromatography
    - Gas
    - Ion Exchange
    - Liquid
  - Combustion and Flames
  - Detonation and Shock Waves
  - Electrochemistry; Polarography
  - Electrolyte Theory
  - Isotope Effects; Isotope Fractionation
  - Isotope Exchange; Isotope Separation
  - Kinetics
  - Photochemistry
    - Flash Photolysis
  - Radiation Chemistry
  - Radiochemistry
    - Positronium Chemistry
- Crystal Field Theory

- Electricity and Magnetism
  - Dielectric Relaxation
  - Electrical Measurements
  - Electromagnetic Theory
  - Electrostatics
  - Magnetic Weighing

METHODS (CONT.)

- Electron Methods
  - Electron Beams
  - Electron Diffraction
  - Electron Scattering; Electron Impact
  - Electron Swarm

- Heat and Thermodynamic Processes
  - Cryoscopy
  - Temperature Measurements
  - Thermal Analysis
  - Classical Thermodynamics
  - Statistical Mechanics; Statistical Thermodynamics
  - Quantum Statistical Mechanics
  - Irreversible Thermodynamics; Non-equilibrium Statistical Mechanics

- Lasers, Masers, and Optical Pumping
- Ligand Field Theory
- Luminescence

- Mathematical Methods
  - Analytical Geometry
  - Differential Equations
  - Group Theory
  - Hilbert Space Theory
  - Statistics
- Mechanics (classical)
- Microscopy
  - Electron Microscopy
    - Field Emission Microscopy
  - Optical Microscopy

- Nucleation

- Optical Methods (Non-spectroscopic)
  - Interferometry
  - Polarimetry
  - Non-linear optics (two-photon processes)
  - Optical Birefringence
  - Polarization
  - Reflection

- Quantum Mechanics
  - Quantum mechanics, general theory
  - Quantum mechanics, methods and calculations
    - Density matrix methods
    - Wave function methods
      - Approximation methods
        - Perturbation theory
          - time-dependent
          - time-independent
        - Variation theory
        - WKB
      - Group theoretical methods

METHODS (CONT.)

        - Ligand field theory
        - Molecular orbital calculations
            - LCAO
            - SCF
            - CI
            - PPP
            - split p
            - electron correlation
            - Huckel
            - MO theories including as well as electrons
    - Quantum mechanics, intermolecular interactions; scattering theory
    - Quantum electrodynamics
    - Field theory

- Scattering
    - Electron Scattering
    - Light Scattering
        - Elastic
        - Inelastic
    - Neutron Scattering
    - Proton Scattering
    - Scattering Theory
    - X-Ray Scattering

- Sorption
    - Absorption
    - Adsorption
    - Desorption

- Transport Processes (see also Statistical Mechanics)
    - Collision Theory; Kinetic Theory of Gases
    - Diffusion
    - Effusion
    - Hydrodynamics
    - Thermal Conduction
    - Thermal Diffusion
    - Transpiration
    - Transport Theory
    - Viscoelastic and Rheological Measurements

DEVICES

- Calorimeters
- Computer Programs
- Counters
- Densitometers
- Dilatometers
- Dosimeters
- Electrodes
- Knudsen Cell
- Magnetometers
- Pressure Gauges; Manometers
- Spectrophotometers
- Viscometers

APPENDIX A
CHEMICAL PHYSICS VOCABULARY

OBJECTS

- Particles
  - Subnuclear
  - Electrons
  - Neutrons
  - Protons
- Nucleus
- Atom
  - Hot
  - Stable
  - Unstable
- Molecule
  - Inorganic
  - Metallo-organic
  - Organic
- Transition-metal complexes and compounds
  - Octahedral
  - Tetrahedral
- Ion
  - Negative
  - Positive

- Catalysts
- Chelates
- Chromophore
- Clathrates
- Dyes
- Electrolytes
- Excitons
- Ferroelectrics
- Free Radicals
- Impurities
- Insulators
- Laser and Maser Materials
- Macromolecules and Proteins
- Metals
- Photoconductors
- Polymers
- Semiconductors

- Fluids
  - Gases
    - Ideal
    - Real
  - Liquids
  - Fluid Mixtures
    - Gas Mixtures
    - Liquid Mixtures and Solutions
- Liquid Crystals
- Solids
  - Crystals
    - Single Crystals
    - Polycrystalline Materials

OBJECTS (CONT.)

- Thin Films
    - Monolayers
    - Multilayers
- Solid Matrix
- Fibers
- Glasses
- Dispersions (colloids)
- Solid Solutions

- Interfaces
- Surfaces

- Non-equilibrium systems and steady states
- Stationary States
- Acid-base systems
- Charge-transfer complexes
- Excited states
- Ion-exchange systems (including proton transfer)
- Ion-molecule interactions
- Polar media
- Singlet state
- Triplet state

- Dipoles
- Electrodes
- Oscillator systems
    - Harmonic oscillators
    - Anharmonic oscillators
- Rotors
    - Non-rigid
    - Rigid
- Spin systems
    - $S=\frac{1}{2}$
    - $S>\frac{1}{2}$
- n-particle systems ($n>3$)
- Three-particle systems

- fat
- hard
- long
- round
- short
- soft
- thin

- cube
- helix
- plate
- random coil
- rod
- sphere
- square
- disc

APPENDIX B

Analysis of Carr–Purcell Spin-Echo NMR Experiments on Multiple-Spin Systems. I. The Effect of Homonuclear Coupling*

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(Received 26 August 1965)

The effect of homonuclear coupling in a molecule on Carr–Purcell spin-echo (CPSE) nuclear magnetic resonance experiments is investigated. A density-matrix approach is used to derive a general equation for the CPSE train of multiple-spin molecules in the liquid state. This general equation predicts a CPSE train modulated with one or more frequencies, whose relative amplitudes are, in general, not equal. Unmodulated contributions may also arise. It is shown that the modulation frequencies and their relative amplitudes are functions not only of the relative chemical shifts and coupling constants, but are strongly dependent on the separation between the 180° pulses, t_{cp}. In addition, the modulation can always be eliminated by making the pulse repetition rate, $1/t_{cp}$, large with respect to all the relative chemical shifts and coupling constants. It is also shown that, for weak coupling, it is possible to derive simplified equations by neglecting the nonsecular part of the coupling Hamiltonian, but this approximation is valid only when $1/t_{cp}$ is of the order of, or smaller than the relative chemical shifts.

Procedures for solving the general equation to obtain closed formulas for the CPSE train of a specific system are discussed. Solutions for spin-½ nuclei are treated in detail. Closed equations are derived for the AB, A_2B, and A_3B systems, and they are used in some numerical calculations. Simplified weak-coupling formulas are also derived for these systems, and their range of validity is discussed.

A very brief discussion of heteronuclear coupling is presented.

J. Chem. Phys. 44, 1 (1966)   Theoretical

Property
Spin-spin coupling
Chemical shift

Object
Molecule
Liquid
Spin system = ½

Method
Nuclear Magnetic Resonance
Density Matrix

J. Chem. Phys. 44, 1 (1966)   Theoretical

Property
Spin-spin coupling
Chemical shift

Object
Molecule
Liquid
Spin system > ½

Method
Nuclear Magnetic Resonance
Density Matrix

Molecular Orbital Theory for Octahedral and Tetrahedral Metal Complexes

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(Received 4 May 1965)

Self-consistent charge and configuration (SCCC) molecular orbital calculations are reported for 32 selected octahedral and tetrahedral first-row transition-metal complexes containing halide and chalcogenide ligands. It is found that for the range of metal oxidation states II through IV, F_σ, chosen to fit the experimental Δ, is a function of only the metal atomic number for constant F_π. In the range of formal metal oxidation numbers V through VII, F_σ is also a function of oxidation number.

Calculated and observed trends in covalency, Δ values, and first L→M charge-transfer energies are compared. The conclusion is drawn that the molecular orbital method, in its present formulation, gives a reasonable account of the ground states and low excited states in simple metal complexes.

J. Chem. Phys. 44, 10 (1966) Theoretical

Property
Charge-transfer energy
Covalence and ionic character
Ionization potential

Object
Transition-metal complexes - octahedral

Method
Ligand field theory

J. Chem. Phys. 44, 10 (1966) Theoretical

Property
Charge-transfer energy
Covalence and ionic character
Ionization potential

Object
Transition-metal complexes - tetrahedral

Method
Ligand field theory

Electronic Spectrum of (2, 2)Paracyclophane. II*

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(Received 16 July 1965)

The studies of the absorption and fluorescence spectra of single crystals of (2,2)paracyclophane in the region 3300–3100 Å reported in a previous paper have been extended. Well-characterized samples with the (*hk*0) developed crystal plane were used. In absorption two distinct spectra were obtained in the two polarization components. The fluorescence was strongly polarized in one direction (parallel to the fourfold *c* axis) and represents the mirror image of the equally polarized absorption component. It was concluded that the observations prove conclusively that the differently polarized spectral components represent transitions to two different electronic states, with an energy difference of 369 cm^{-1}. The lowest-energy transition certainly contains the 0–0 line and all available evidence supports the conclusion that also the second transition has allowed character. The only interpretation consistent with all observed features of the spectra is as follows. The two observed states are the gerade dimer states (B_{2g} and B_{3g} in D_{2h}) being the out-of-phase combinations of the B_{2u} and B_{1u} benzene moiety states. The transitions have allowed character due to a torsional distortion of the molecule in the excited state. The interpretation is fully consistent with theoretical energy calculations.

J. Chem. Phys. 44, 19 (1966 Experimental

Property
Luminescence spectra
Electronic spectra
Torsional energy

Object
Crystal, single
Molecule, organic $C_{16}H_6$
Excited state

Method
Ultraviolet and visible spectroscopy
Densitometer

3100 - 3300 Å.

-NSF

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