SHORYGIN, P. P. and YEGOROVA, Z. S.

"On Relation of Spectra to Angle of Twist of Methoxy and Dimethylamino Groups with respect to Benzene Ring Plane."

report presented at the 4th International Meeting of Mclecular Spectroscopy, Bologna, Italy, 7-12 Sept 1959.

Institute of Physical Chemistry, the University of Moscow.

SHORYGIN, P.P.; ALAUNE, Z.B. [Alaune, Z.]

Optical research of the interference of atomic groups in the molecules of organic compounds. Liet ak darbai B no.4:57-69 '59.

1. Institut organicheskoy khimii im. N.D. Zelinskogo AN SSSR i Institut khimii i khimicheskoy tekhnologii AN Litovskoy SSR.

(Organic compounds) (Molecules)

(Atoms)

5(4), 5(3)

AUTHORS:

Shorygin, P. P., Alaune, Z. B.

SOV/76-33-3-33/41

TITLE:

Investigation of Solutions of Aromatic Amines in Organic Acids (Issledovaniye rastvorov aromaticheskikh aminov v

organicheskikh kislotakh)

PERIODICAL:

Zhurnal fizicheskoy khimii, 1959, Vol 33, Nr 3, pp 717-721

(USSR)

ABSTRACT:

In the case of aromatic compounds which possess an electronegative group in the para-position to the amino group, a salt formation leads to a noticeable variation of the absorption spectrum. Similar variations may be stated by comparing the Raman spectra of nitro-benzene solutions with p-nitro-dialkyl aniline. According to these data the authors of a previous paper (Ref 1) assumed that in acetic acid solutions aniline (I) forms no salt but a compound with the solvent. In this case the authors studied the spectra of the solutions of (I) and dimethyl aniline (II) as well as the corresponding para-nitro compounds. The absorption spectra were obtained by means of the photoelectric spectro-

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photometer SF-4 with a concentration of 10^{-2} - 10^{-4} moles/1 of the substances under investigation. The Raman spectra were photo-

504/76-33-3-33/41

Investigation of

Solutions of Aromatic Amines in Organic Acids

graphed by means of the three-prism spectrograph ISP-51 with the excitation of the Hg line 4358 A (concentrations of (I) and (II) being about 10%, that of p-nitrodiethyl aniline (III) being $\langle 1\% \rangle$. On the basis of the absorption spectra obtained from (I) in acetic acid (IV), heptane and HCl solutions (Fig 1) it is assumed that a salt was formed by about 95% (I) in 80% acetic acid. Since (I) is acetylated already at room temperature, the Raman spectra of the system (I) + (IV) cannot be clearly interpreted. (II) is not acetylated and it was possible to determine the coefficients of the line intensity of the benzene ring (I_{1600}/I_{1000}) for (II) (Table). The absorption curves of the solutions of (II) (Fig 2) indicate that up to 90% of salt is formed in 100% acetic acid. The above-mentioned spectroscopic data, however, do not exclude the formation of complex compounds. The absorption spectra c1 (III) show (Fig 3) that no special salt formation occurs in acetic acid, whereas in a benzene solution of trichloro acetic acid 99% of (III) pass into a salt. There are 3 figures,

Card 2/3

1 table, and 3 Soviet references.

SOV/76-33-3-33/41

Investigation of the Solutions of Aromatic Amines in Organic Acids

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Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physical and Chemical Institute imeni L. Ya. Karpov)

SUBMITTED: September 11, 1957

Card 3/3

ASSOCIATION:

.5 (4) AUTHOR:

Shorygin, P. P.

sov/76-33-7-6/40

CITLE:

Mutual Influence of Substituents in the Molecules of the

p-Disubstituted Derivatives of Benzene

PERIODICAL:

Zhurnal fizicheskoy khimii, 1959, Vol 33, Nr 7, pp 1477 - 1483

(USSR)

ABSTRACT:

All experiments failed which have hitherto been made for the purpose of describing chemical and physical properties of the benzene derivatives by independent constants or increments (which characterize the substituents, as, for example, data on absorption spectra (Ref 1)). In order to form an idea of the properties of aromatic compounds with two substituents, the author compared here the results of an investigation of three types of compounds (X-C₆H₅, NO₂-C₆H₄-X, and X-C₆H₄-NR₂) (Table).

He referred to data available in publications on dipole moments and spectra as well as to data published in the preceding papers (Refs 3.5) and (Ref 4). The table shows the influence exercised by the NO₂- and NR₂ group upon the frequency of oscillation of

the individual substituents X. The latter are divided into

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* Mutual Influence of Substituents in the Molecules of SOV/76-33-7-6/40 the p-Disubstituted Derivatives of Benzene

4 groups (in the table), one group with distinctly marked electronegative properties and another with electropositive properties. These considerations led to the following conclusions: The difference in the ability of the substituents X to act as electron denors is greater in the dipole moments of $^{\rm p-XC}6^{\rm H}4^{\rm NO}2^{\rm p}$ smaller in the dipcle moments of $^{\rm c}6^{\rm H}5^{\rm X}$, and still smaller in the dipole moments of p-XC $_{6}^{H}{}_{4}^{NR}{}_{2}^{}$. The ability to art as electron donors of the substituents depends on the kind of mutual influence of the groups of atoms and cannot be tharacterized by an independent increment. The introduction of the individual substituents X results almost in all cases in an approximation and intensification of the neighboring intense absorption waves. The influence exercised by the substituents upon the physical and chemical properties of p-XC $_6^{\rm H_4Y}$ molecules is stronger if one of the substituents is electronegative and the other electropositive, and it is considerably weaker if both substituents are electropositive or electronegative. The sequence of the substituents in the order of their influence

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Matual Influence of Substituents in the Molecules of SOV/76-33-7-6/40 the p Disubstituted Derivatives of Benzene

> upon the individual properties of the molecules offers many General data, a definite relationship, however, is not to be expected. Some discussions are given concerning the reasons for the differences in this sequence. There are 5 figures; table, and 14 references, 4 of which are Soviet.

ASSOCIATION: Institut organicheskoy khimii AN SSSR, Moskva (Institute of

Organic Chemistry of the AS USSR: Moscow)

SUBMITTED: September 11, 1957

Card 3/3

5.3610,5.3100

77082 SOV/62-59-12-26/43

AUTHORS:

Shorygin, P. P., Shkurina, T. N., Shostakovskiy, M. F.,

Sidel kovskaya, F. P., Zelenskaya, M. G.

TITLE:

Spectroscopic Investigation of N-Vinyllactams and

Anilides

PERIODICAL:

Izvestiya Akademii nauk SSSR. Otdeleniye khimicheskikh

nauk 1959, Nr 12, pp 2208-2212 (USSR)

ABSTRACT:

Spectra of N-vinyllactams and anilides were studied, and the mutual influence of groups was investigated. Vinyllactams contain the system C=C-N-C=O; the examination of the interaction of atoms and groups can be simplified, to the first approximation, by considering the effect of the N-atom on C=C and C=O bonds, as well as the mutual interaction of the double bonds. Raman and UV-spectra of vinylpyrrolidone, vinylpiperidone, vinylcaprolactam, of various anilides (formanilide, acetanilide, etc.), and of simpler molecules containing an N-atom and a carbonyl group (pyrrolidone, N-butylpyrrolidone,

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caprolactam, dimethylacetamide were taken. Spectrograph

Spectroscopic Investigation of N-Vinyllactams and Anilides

77082 SOV/62-59-12-26/43

ISP-51 and PRK mercury lamp were used to obtain Raman spectra, and spectrograph SF-4 to obtain UV-spectra. Spectra of vinyllactams in the double bonds region showed lines characteristic for C=C and C=O bonds. It was found that the presence of the N-atom at the double bond influenced considerably the spectral characteristics: the frequency of the C=0 bond was lowered nearly as much as in molecules containing N-C=0 bonds. Values of the extinction coefficient of C=0 bond line in vinylpiperidone and vinylcapro lactam were quite high, and close to those of vinylamine. The intensity of C=C line of vinylpyrrolidone was substantially higher, and that of C=0 line in all three vinyllactams was many times higher than in compounds with > N-C=0 bonds. This anomaly in the intensity of the C=0 bond in Raman spectrum was the most peculiar characteristic of vinyllactams which distinguished them from molecules with C = C - N < and N-C=0 bonds. It can be explained by the influence of the C=C bond, through the N-atom, on the carbonyl group (in the bond system C=C-N-C=0). Similar

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Spectroscopic Investigation of N-Vinyllactams and Anilides

77082 SOV/62-59-12-26/43

relationships were also observed in anilide spectra. It was noted that the alkylation of N in anilides weakened the indications of conjugation of N with the benzene ring, and strengthened those of conjugation with the carbonyl group. It can be assumed, therefore, that a C₆H₅NRCO·X molecule loses the coplanarity of the system C₆H₅-N-C and the system C-N-COX becomes more planar. There are 3 tables; 1 figure; and 6 references, 1 U.S., 1 U.K., 1 German, 3 Soviet. The U.S. and U.K. references are R. Bowden, E. Braude, E. Jones, J. Chem. Soc., 1946, 948; E. Corey, J. Amer. Chem. Soc., 75, 2301 (1953).

ASSOCIATION:

N. D. Zelinskiy Institute of Organic Chemistry, Academy of Sciences, USSR (Institut organicheskoy khimii imeni N. D. Zelinskogo Akademii nauk SSSR)

SUBMITTED:

April 7, 1958

Card 3/3

24(7)

AUTHOR: Shorygin, P.P., Professor

s/030/60/000/01/022/067

B015/B008

TITLE:

4th International Conference on Molecular Spectroscopy

PERIODICAL:

Vestnik Akademii nauk SSSR, 1960, Nr 1, pp 68-70 (USSR)

ABSTRACT:

The Conference was convened by the International Association for Theoretical and Applied Chemistry in Bologna (Italy) in September 1959. More than 500 scientists attended, among them 14 from the Soviet Union. More than 200 reports were received which dealt with a wide range of problems of molecular spectroscopy. The Soviet scientists gave reports dealing with the individual trends developed in Soviet spectroscopic laboratories. On the recommendation of the Scientific Faculty of Bologna University, the medal G. Ciamiciano was awarded to A.N. Terenin, Soviet Scientific Academician, for outstanding studies in the field of spectroscopy. An exposition of optical instruments was combined with the Conference, among which the double beam spectrophotometer of type CF-41 (see figure) and the double beam vacuum appliance of type IR-7 (see figure) are specially mentioned. The Conference stressed the increasing

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APPROVED FOR RELEASE: 08/09/2001 CIA-RDP86-00513R001549910012-9"

significance of molecular spectroscopy. There are 2 figures.

68849 s/076/60/034/02/011/044 5.3100 Shorygin, P. P., Geyderikh, M. A., B010/B015 AUTHORS: Ambrush, T. I. The Effect of Substituents on the Properties of Aromatic Nitriles TITLE: and Sulfones 1 Zhurnal fizicheskoy khimii, 1960, Vol 34, Nr 2, pp 335-342 (USSR) The Raman spectra, ultraviolet absorption spectra, and dipole PERIODICAL: moments of the para-derivatives of benzonitrile and methylphenylsulfone were examined and compared. The frequency values of the ABSTRACT: Can-group valence oscillation of the para-derivatives of the benzonitrile Raman spectrum, of the coefficients of integral intensity ICN of the CN line in the Raman spectrum, of the intensity ion of the CN absorption band in the infrared spectrum, of the wave lengths of the most important maxima of the intensive absorption bands in the ultraviolet spectrum (measured with the SF-4 spectrophotometer), and the dipole moments (measured by V. N. Vasil'yeva and Z. S. Yegorova in benzene and dioxane) are shown by table 1. Table 2 shows the frequency difference of the groups Y in the molecule $X \leftarrow Y$ and $Y = NO_2$, COR, CN, SOOR, OE), as well as the corresponding wave length difference ΔX of the card 1/3

The Effect of Substituents on the Properties of Aromatic Nitriles and Sulfones

S/076/60/034/02/011/044 B010/B015

absorption bands, and the difference between the measured dipole moment for X-Y and the vector sum of the moments for $X \leftarrow A$ and $A \leftarrow A$ The effect of substituents exerted on the investigated properties of the nitro compounds, ketones, nitriles, and sulfones is of the same character. The order of substituents (corresponding to the effect on the mentioned properties) is approximately the same for the four types of compounds mentioned. In this respect, sulfones do not differ from nitro compounds. The effect of substituents is, however, strongest with nitro compounds, and weakest with sulfones (Table 2). The electropositive substituents reduce the frequency of NO2, CN, CO, and SO2, increase, however, that of OH. The OR group influences the optical properties of the compounds investigated more strongly than the OH group whereas the dipole moments and dissociation constants of phenols and acids are more strongly influenced by the OH group. The assumption put forward in publications that the SO2 group is incapable of forming a conjugation is unfounded. The difference in the ICN values of some nitriles is in qualitative agreement with the difference in the ich values. V. A. Petukhov took some of the

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The Effect of Substituents on the Properties of Aromatic Nitriles and Sulfones

S/076/60/034/02/011/044 B010/B015

absorption spectra. There are 2 figures, 3 tables, and 9 references, 2 of which are Soviet.

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ASSOCIATION:

Institut organicheskoy khimii AN SSSR (Institute of Organic Chemistry of the AS USSR)

SUBMITTED:

April 26, 1958

Card 3/3

ShoryGin, P.P.

S/020/60/133/02/23/068 B019/B060

AUTHORS:

Shorygin, P. P., Krushinskiy, L. L.

TITLE:

On the Theory of Combination Scattering of Light?

PERIODICAL:

Doklady Akademii nauk SSSR, 1960, Vol. 133, No. 2,

pp. 337-340

TEXT: By way of introduction, the authors derive the classical formula (1) and the quantum-theoretical formula (3) for the calculation of the spectral lines of combination scattering. The applicability of these formulas is discussed, and formula (1) is graphically illustrated in formulas is diagram holds for the classical model of a diatomic molecule Fig. 1. This diagram holds for the classical model of a diatomic molecule with excited states of short lifetime. Similar results are obtained for the quantum-theoretical model, as follows from the analogous diagram in Fig. 2. From the discussion of the formulas derived here and from the diagrams shown the authors conclude that with a decrease in the diagrams shown the higher harmonic an approach occurs to that intensity distribution which is observed with resonance fluorescence. Some experimental data are discussed, and it is shown that the intensity of

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On the Theory of Combination Scattering of Light

S/020/60/133/02/23/068 B019/B060

the lines does not, as often stated, change proportionally with absorption. The observation of a resonance Raman spectrum is said to be restricted by the large absorption losses of light (up to 99% and more). However, the authors note from formulas (1) and (3) that in the region of the strongest absorption bands the conditions for the observation of a resonance scattering are considerably more favorable than in the region of weaker bands. There are 3 figures and 2 Soviet references.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physico-chemical Institute imeni L. Ya. Karpov)

PRESENTED:

March 3, 1960, by I. V. Obreimov, Academician

SUBMITTED:

February 29, 1960

Card 2/2

VC

25039 \$/062/61/000/006/001/010 B118/B220

5.3400

Shorygin, P. P., Shkurina, T. N., Shostakovskiy, M. F., and

Gracheva, Ye. P.

TITLE:

- AUTHORS:

Spectra and structure of vinyl ethers

PERIODICAL:

Akademiya nauk SSSR. Izvestiya. Otdeleniye khimicheskikh

nauk, no. 6, 1961, 1011 - 1015

TEXT: A study has been made of the influence of various functional groups on the properties of vinyl compounds and on the state of the double bond C=C. In the case of vinyl ethers, the influence exerted by the alkoxy group upon the double bond becomes evident in chemical properties, such as increased reactivity in addition reactions, in hydrolysis, and in polymerization and copolymerization processes. Not much material is available in the literature with regard to the influence of the alkoxy group upon the strength of the double bond C=C and upon the optical properties. The present paper deals with studies concerning the Raman spectra and the ultraviolet absorption spectra in vacuo for a series of vinyl ethers containing alkyl, naphthene and aromatic radicals. Most vinyl ethers

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Spectra and structure of ...

have several lines in the frequency range of the stretching vibrations C=C. The splitting depends on the branchings of the alkyl group and on the presence of an &-substituent. The influence of temperature upon the intensity of the lines ~1610 and ~1640 cm⁻¹ of vinyl butyl ether indicates their relation to the two rotational isomers. The influence of the group OAlk on $\omega_{\text{C=C}}$ may be regarded qualitatively as a tendency to reduce the frequen-The wavelength of the first absorption band and the intensity of the C=C line in the Raman spectra are greater for vinyl ethers than for alkenes of similar structure. The influence of solutions and temperature on the structure of the C=C band was studied. Thus, the geometric configuration of the molecules of vinyl ethers may be important to both the physical and chemical properties. The Raman spectra were taken with the NCT-67 (ISP-67) spectrograph with the Hg line 4358A. The absorption spectra were taken with spectrophotometers of types C Φ -4 (SF-4) and C Π -41 (SP-41) with the assistance of V. A. Petukhov. There are 2 figures, 1 table, and 3 references: 1 Soviet-bloc and 2 non-Soviet-bloc. The 1 reference to English-language publication reads as follows: Y. Mikawa, Bull. Chem. Soc. Japan 29, 110 (1956).

Card 2/6

25039 s/062/61/000/006/001/010 B118/B220 Spectra and structure of ... Institut organicheskoy khimii im. N. D. Zelinskogo Akademii ASSOCIATION: nauk SSSR (Institute of Organic Chemistry imeni N. D. Zelinskiy of the Academy of Sciences USSR) SUBMITTED: June 1, 1959 Fig. 1: Ultraviolet absorption spectra of octene-1 and vinyl ethers (solutions in heptane). Legend: bu-butyl group; - - - - cyclohexyl group. Card 3/6

SHORYGIN, P.P.; SHOSTAKOVSKIY, M.F.; PRILEZHAYEVA, Ye.N.; SHKURINA, T.N.; STOLYAROVA, L.G.; GENICH, A.P.

Structure and spectra of vinyl sulfides. Izv. AN SSSR. Otd.khim.nauk no.9:1571-1577 S '61.

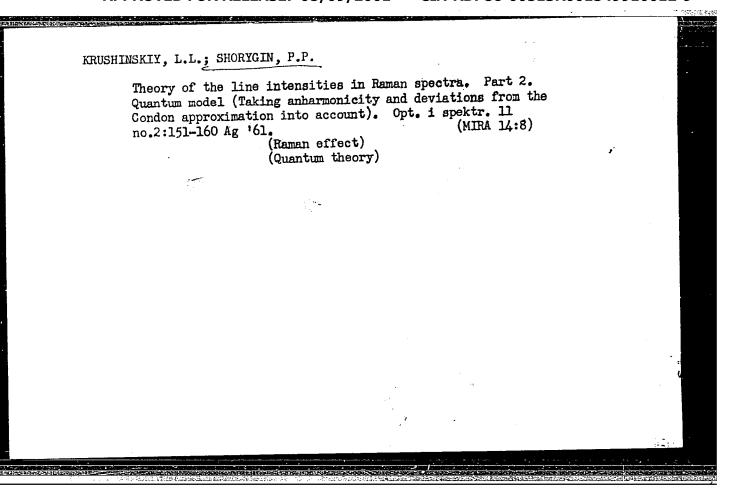
1. Institut organicheskoy khimii im. N.D.Zelinskogo AN SSSR. (Vinyl sulfide--Spectra)

Theory of line intensities in light scattering spectra. Fart 1.

Quantum model (Conion approximation). Opt.i spektr. 11 mo.l:24-34

Jl '61.

(Raman effect) (Quantum theory)



S/076/61/035/002/002/015 B124/B202

AUTHORS: Shorygin, P. P., Roshohupkin, V. P., Petukhov, V. A., and

Yegorova, Z. S.

TITLE: Effect of substituents on the properties of molecules

containing a system of conjugate π bonds

PERIODICAL: Zhurnal fizicheskoy khimii, v. 35, no. 2, 1961, 258-268

TEXT: The authors study the group of para-derivatives of nitrobenzene $X- \bigcirc -NO_2$ with different substituents X. To characterize the compounds the following values are given in Table 1: 1) difference $(\Delta \omega_s$, in cm⁻¹) between the values of symmetrical stretching vibrations of the nitro group of the compound $X- \bigcirc -NO_2$ and those of non-

substituted nitrobenzene on the basis of the Raman spectra of benzolic solutions; the accuracy is $^+$ 0.5 - 1cm⁻¹ (the values with asterisks are obtained from the infrared spectra). In the case of doublets the mean value of the frequency which has the symbol \sim is given. The frequency

Card 1/9

s/076/61/035/002/002/015

B124/B202 Effect of substituents on the properties ... ω_s of the nonsubstituted nitrobenzene in benzene is 1347.5 cm⁻¹; 2) the difference $(\Delta \omega_{as} \text{ in cm}^{-1})$ between the values of the frequency of the antisymmetric stretching vibration of the nitro group of compound angle- NO $_2$ and of those of nitrobenzene on the basis of the infrared absorption spectra of the benzolic solutions; accuracy ± 2 cm⁻¹. The frequency ω_{as} of nitrobenzene is 1533 cm⁻¹; 3) the coefficient of the total intensity (Is) of the Raman bands with the frequency ω_s ; 4) characteristics of the intense absorption bands in the UV range for solutions in heptane; the wavelengths are given in parentheses in A; at the values $\varepsilon/1000$, ε denotes the (decimal) molar absorption coefficient in the maximum of the bands; 5) difference (λ_1 , in A) between the λ_1 -values of the compounds X - \sim - NO₂ and those of nitrobenzene from the values measured in benzene; 6) difference ($\Delta\mu$) between the dipole moment μ of . compound X - NO2 and the sums of the vectors of the moments \bigcirc NO $_2$ (in debyes) which alsocharacterize the interaction Card 2/9

S/076/61/035/002/002/015 B124/B202

Effect of substituents on the properties...

of the groups concerned, and 7) Hammett constants $\sigma_{\hbox{para}}$ characterizing the effect of the substituents X on the reactivity of the groups Y in the molecules X - O - Y. The electropositive and electronegative substituents influence the oscillation frequency of the nitro group as well as the deviations of the dipole moments from the additivity and the reactivity mainly in opposite direction, whereas they influence the optical properties (intensity of Raman bands of the NO2 group, polarizability, position and intensity of the absorption bands) in the same direction. In all cases, the effect of the electropositive substituents in the molecules X - - NO2 is considerably stronger than that of the electronegative substituents, whereas the opposite holds for the molecules. Ramified and not ramified alkyl groups influence the physical properties of the nitro compounds in the same way. The effect of methylation on the influence of the substituents increases in the following order: CH2 < OH < SH < NH2. The effect of the substituents C6H5 and CH2: CH2 on the dipole moments, frequency of the nitro groups, and the chemical properties is relatively low, on the optical properties, however, it is strong. This holds for substituents of the type CH:CH.Z, .C6H4.Z and .N:N.Z.

Card 3/9

S/076/61/035/002/002/015 B124/B202

Effect of substituents on the properties...

interaction of two atom groups on their chemical bonds is reduced with increasing length of the chain of the π bonds which separate these groups from one another. The effect of the substituents on the optical properties is the stronger the longer the chain of the conjugate bonds. Heavy atoms which are connected with the system of π bonds over a CH₂ bridge considerably influence the system concerned, i.e., mainly the parameters of the electron excitation levels. T. I. Ambrush, M. A. Geyderikh, Ye. A. Smirnov, A. V. Dombrovskiy, E. I. Budovskiy, G. S. Ter-Sarkisyan, U. I. Khurgin, A. Kh. Khomenko, A. N. Nesmeyanov, R. V. Golovnya, B. V. Lopatin, V. N. Vasil'yeva, and V. G. Vasil'yev are mentioned. There are 6 figures, 1 table, and 3 references: 2 Soviet-bloc and 1 non-Soviet-bloc. 1 reference to English language publications reads as follows: C. Curran, F. Palermiti, J. Amer. Chem. Soc. 73, 3733, 1951.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physico-

chemical Institute imeni L. Ya. Karpov); Institut

organicheskoy khimii AN SSSR (Institute of Organic Chemistry

AS USSR)

SUBMITTED:

April 11, 1957

Card 4/9

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S/076/61/035/002/002/015 B124/B202

Effect of substituents on the properties

Legend to Table 1: 1) group X in, 2) stretching vibrations in the nitro group, 3) UV absorption spectra..., 4) σ_{para} , 5) ferrocene. The methyl group is designated with R in the formulas, the H-atoms at the carbon are omitted in most of the formulas; the hexagon or Ph denote the benzene ring. λ , ϵ and f (oscillator output) are given for solutions in heptane and $\Delta\lambda_1$ for solutions in benzene; λ_1 of the non-substituted nitrobenzene in benzene is 2620 A approximately; + are the absorption bands with fine structure; the tables give the values λ and ϵ of the most intense component. The position of the inflection point of the absorption curve is given in brackets.

Card 9/9

\$/020/61/136/003/012/027 B019/B056

24.4500

AUTHORS:

Krushinskiy, L. L. and Shorygin, P. P.

TITLE:

Consideration of the Oscillating Structure of the Electron Excitation Levels of Molecules in the Quantum Theory of

Light Scatter

PERIODICAL:

Doklady Akademii nauk SSSR, 1961, Vol. 136, No. 3,

pp. 577-580

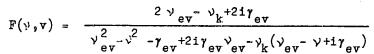
TEXT: An important part of the quantum theory of light scatter by molecules is taken up by the analysis of the contribution of oscillation sublevels in the polarizability matrix elements determining the line intensities in the spectrum. If as contribution of the v-th sublevel of the electron excitation level of the investigation to the polarizability matrix element a^{mn} (corresponding to the vibrational transition $m \longrightarrow n$) the quantity

 $A_{v}^{mn} = F(v,v) \langle v|M_{oe}(r)|m \times v|M_{oe}(r)|n \rangle$ (1) is considered, where

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Consideration of the Oscillating Structure of the Electron Excitation Levels of Molecules in the Quantum Theory of Light Scatter

S/020/61/136/003/012/027 B019/B056



is a frequency factor, γ_{ev} - the frequency of transition to the v-th sublevel of the excited state from the m-th sublevel of the ground state, γ_{ev} - the width of the v-th sublevel, γ_k the frequency change of a photon in scattering, γ - the frequency of the exciting light, $M_{oe}(\mathbf{r})$ - the momentum matrix element, developed from the electron wave function, and \mathbf{r} the internuclear distance. Thus, the polarizability matrix element

may be given with $a^{mn} = \frac{1}{hc} \sum_{v} A_{v}^{mn}$ (2). The relation (2) may be obtained from the Kramers-Heisenberg formula, if the complete wave function of a bi-atomic molecule is investigated in adiabatic approximation. The authors confine themselves for simplicity's sake to an excitation level

Card 2/5

Consideration of the Oscillating Structure S/020/61/136/003/012/027 of the Electron Excitation Levels of Molecules B019/B056 in the Quantum Theory of Light Scatter

and investigate only the diagonal elements of the polarizability tensor. In first approximation

 $M_{oe}(r) = M_{oe}^{o}(1 + \eta r) \quad (6) \text{ is obtained, and thus from formula (1) the}$ $expression \quad A_{v}^{mn} = F(v,v)(M_{oe}^{o})^{2} \left\{ (v,m) + \eta(v,rm) \right\} \left\{ (v,n) + \eta(v,rn) \right\} \quad (7)$

is derived, where $(v,rm) = \langle v|r|m \rangle$. For the contributions of the

sublevels in the equation $A_v^{mn} = F(v,v)M_{oe}^2B_v^{mn}$ the following expressions are obtained by Condon approximation:

$$B_{v}^{\circ \circ} = \frac{1}{v!} \left(\frac{\alpha \Delta^{2}}{2} \right)^{v} \exp\left(-\frac{\alpha \Delta^{2}}{2} \right) \left\{ \left(1 + \gamma \vec{r}_{o} \right) - \frac{\gamma}{\alpha \Delta} \right\}^{2}$$

$$B_{v}^{01} = \frac{1}{v!} \left(\frac{\alpha \Delta^{2}}{2}\right)^{v-1/2} \exp\left(-\frac{\alpha \Delta^{2}}{2}\right) \left(\frac{\alpha \Delta^{2}}{2} - v\right) \cdot \left\{ (1+\eta \bar{r}_{0}) (1+\eta \bar{r}_{0} + \frac{\eta}{\alpha \Delta}) \right\}$$

Card 3/5

Consideration of the Oscillating Structure of the Electron Excitation Levels of Molecules in the Quantum Theory of Light Scatter

S/020/61/136/003/012/027 B019/B056

$$-\frac{\eta}{\alpha\Delta}\left(2+2\eta\bar{r}_{0}+\frac{\eta}{\alpha\Delta}\right)v+\frac{\eta^{2}}{\alpha^{2}\Delta^{2}}v^{2}$$

$$B_{v}^{02} = \frac{\sqrt{2}}{2} \frac{1}{v!} \left(\frac{\alpha \Delta^{2}}{2}\right)^{v-1} \left\{ \left(\frac{\alpha \Delta^{2}}{2}\right)^{2} - 2v\frac{\alpha \Delta^{2}}{2} + v(v-1) \right\} \exp\left(-\frac{\alpha \Delta^{2}}{2}\right)$$

$$\times \left\{ (1+\eta \bar{r}_{0})(1+\eta \bar{r}_{0}+\frac{\gamma}{\alpha \Delta}) - \frac{2\eta}{\alpha \Delta}(1-\eta \bar{r}_{0}+\frac{\gamma}{\alpha \Delta})v + \frac{\gamma^{2}}{\alpha^{2}\Delta^{2}}v^{2} \right\}.$$

It is further stated that the representation of $M_{Oe}(r)$ with (6) is permitted only in a small interval r which, however, is sufficiently large for calculating (v,rm). If the function $M_{Oe}(r)$ within this range does not change its sign, the Condon approximation represents the contribution of the sublevels. In the opposite case, these contributions of the sublevels change more or less considerably and a bifurcation of the absorption band may occur. Thus, for instance, at $v = E\left\{(\alpha \Delta/\gamma)(1+\gamma r_O^*)\right\}$ the expression

Card 4/5

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Consideration of the Oscillating Structure S/020/61/136/003/012/027 of the Electron Excitation Levels of Molecules B019/B056 in the Quantum Theory of Light Scatter

for $B_v^{00} \cong 0$. These relations are finally discussed in detail. There are 1 figure and 6 references: 3 Soviet and 2 German.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova (Institute

of Physics and Chemistry imeni L. Ya. Karpov)

PRESENTED: July 21, 1960, by A. N. Terenin, Academician

SUBMITTED: July 12, 1960

Card 5/5

Unusual manifestations of the mutual influence of atomic groups in spectra of complex molecules. Dokl. AN SSSR 146 no.5:1132-1135 (MIRA 15:10) 0 162. (Chemical bonds) (Organic compounds-Spectra)

SHORYGIN, P.P.; KRUSHINSKIY, L.L.

"LICHTSTREUNG, FLUORESZENZ UND ERSCHEINUNGEN DES ZWISCHENTYPS."

Report presented at the Spectrascopicum, 11th Intl. Called, Belgrade, Yug, 30 Sep - 4 Oct 63.

MAGGINERATY, L. L.; SHORYGIN, P. P.

"Sur la Correspondance des Resultats de la Theorie de L'Effect Raman Classique et Quantique."

report submitted to 11th Intl Spectroscopy Colloq, Belgrade, 30 Sep-4 Oct 63.

Inst Organic Chemistry, AS USSR, Moscow.

SHORYGIN, P.P.; IVANOVA, T.M.

Raman effect and the lifetime of an excited state. Opt. i spekt. 15 no.2:176-181 Ag '63. (MIRA 17:1)

PETUKHOV, V.A.; MIRONOV, V.F.; SHORYGIN, P.P.

Ultraviolet spectra and structure of unsaturated compounds of the elements of group IV. Izv. AN SSSR Ser. khim. no.12:2203-2206 (MIRA 18:1)

1. Institut organicheskoy khimii imeni N.D. Zelinskogo AN SSSR.

KRUSHINSKIY, L.L.; SHORYGIN, P.P.

Theory of line intensities in Raman spectra. Part 5. Opt. i spektr. 16 no.1:30-39 Ja '64. (MIRA 17:3)

KRUSHINSKIY, L.L.; SHORYGIN, P.P.

Some aspects of the classical theory of the resonance transformation of light by molecules. Izv.AN SSSR.Ser.fiz. 27 no.4: 497-502 Ap 163. (MIRA 16:4) (Oscillators, Electric) . (Nuclear optical models)

<u>L 10833-63</u> EWP(1)/EWT(1)/EWT(m)/BDS--AFFTC/ASD--Pc-4--RM ACCESSION NR: AP3000747 S/0020/63/150/003/0533/0536

AUTHOR: Shorygin, P. P .: Ivanova, T. M.

TITLE: Molecular light scattering and lifetime of excited states

SOURCE: AN SSSR. Doklady, v. 150, no. 3, 1963, 533-536

TOPIC TAGS: Raman effect, lifetime of excited states, band spectra, diphenyl-polyenes, fluorescence of organic molecules

ABSTRACT: The purpose of this study was the elucidation of the interaction between light and molecules. The Raman spectra of compounds with a large lifetime of electron-vibrational energy levels can give the intensity of the fundamental frequency and of overtones, the widths of the lines, and the degree to which the normal vibrations are the same in the absorption-, scattering, and fluorescent spectra. The resonance Raman spectra of the diphenylpolyenes Ph-(CH=CH) sub n -Ph were studied in this work, particularly those of diphenyldecapentaene Ph-(CH=CH) sub 5 - Ph and diphenyldecahexaene Ph-(CH=CH) sub 6 -Ph in an acetone solution which were excited with Hg-lines of wave numbers of 24,705 and 22,938 cm sup -1. The experimental curves for the absorption coefficient vs. the wave number as well as the Raman and fluorescence spectra for these two compounds are given. The

Card 1/2

L 10833-63

ACCESSION NR: AP3000747

spectra were obtained at 25C; the absorption spectra at -70C and the secondary spectra at -196C are also given. At a lower temperature, the intensity of these Raman spectra changes much more than in the non-resonance spectra. This is attributed to the increase of the lifetime of the corresponding levels and to the shift of the absorption bands. Other peculiarities of the secondary spectra are also described. Orig. art. has: one figure and two tables.

ASSOCIATION: Institut organicheskoy khimii im. N. D. Zelinskogo Akademii Nauk SSSR (Institute of Organic Chemistry, Academy of Sciences SSSR)

SUBMITTED: 24Dec62

DATE ACQD: 21Jun63

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NO REF SOV: 004

OTHER: 003

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UR/0058/65/000/003/D015/D015 EMT(1) L 49777-65 AR5012238 ACCESSION NR: SOURCE: Ref. zh. Fizika, Abs. 3Dl04 AUTHORS: Krushinskiy, L. L.; Shorygin, P. P. TITLE: Concerning the correspondence between the results of quantum and classical theory of the intensity of Raman lines AN SSSR, vyp. 1, 1964, 162-169 CITED SOURCE: Tr. Komis. po spektroskopii. TOPIC TAGS: optical center, quantum theory, classical theory, correspondence principle, Raman scattering, Raman line TRANSLATION: Different optical center models used in the theory of Raman scattering are compared. The quantum model considered is a system with two electon-energy levels possessing a vibrational structure (the molecular wave functions are chosen in the Born-Oppenheimer approximation). The classical models used are linear operators: a) with periodically varying parameters; b) with adiabatically slowly varying parameters. The regions of correspondence between the quantum and classical Card 1/2

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L 12906-65 EWT(1)/EEC(b)-2 IJP(c)/AFWL/ASD(m)-3/SSD/ESD(gs)/ESD(t)

ACCESSION NR: AP4047176

s/0051/64/017/004/0551/0557

AUTHORS: Shory*gin, P. P.; Krushinskiy, L. L.

В

TITLE: Interrelation between light scattering and <u>fluorescence</u>, and transition phenomena

SOURCE: Optika i spektroskopiya, v. 17, no. 4, 1964, 551-557

TOPIC TAGS: light scattering, fluorescence, resonance spectrum, molecular spectrum, resonance scattering, nonresonant scattering

ABSTRACT: It is shown that the energy distribution in the spectrum of secondary radiation of light from molecules can be described both on the basis of quantum and on the basis of the classical model of a light-scattering molecule. The simple classical model is more suitable for the excitation of Raman spectra away from resonance, where it can explain adequately the connection between the intensity of the Raman lines and the main parameters of the electronic absorp-

Card 1/3

L 12906-65 ACCESSION NR: AP4047176

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tion spectra. It is also suitable under resonance conditions, provided the oscillator attenuation constant (γ) is much larger than the frequency ω of the nuclear oscillations. When $\gamma >> \omega > \Gamma$ (the half-width of the radiation incident on the molecule) resonance scattering differs from the nonresonance scattering principally in having a larger line intensity. When $\omega > \gamma > \Gamma$, it becomes necessary to use the quantum approach. The line intensity distribution comes closer to that of resonance fluorescence, but the line contours retain the specific features of scattering. When $\omega > \gamma \simeq \Gamma$ the line contours lose all similarity to the contour of the incident-light line, and when $\Gamma > \gamma$ the radiation acquires all the features of resonance fluorescence. When the quantum approach is used, such a classical concept as the polarizability must be replaced by a concept of a transfer function for the quantum oscillator. Orig. art. has: 5 formulas and 2 figures.

ASSOCIATION: None

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Skercoll, i.r.; FORCY, Ye.M.

Characteristics of the vechanical properties of chamical bonds in polyatomic molecules. Zhur. fiz. Zhim. 38 no.6:1/29-1/33 Je 164.

1. Institut organicheskoy khimii AN SSSR.

s/0020/64/154/003/0571/0574

AUTHORS: Shory*gin, P.P.; Krushinskiy, L.L.

ACCESSION NR: AP4013327

TITLE: Light scattering, florescence, and transient phenomena

SOURCE: AN SSSR. Doklady*, v. 154, no. 3, 1964, 571-574

TOPIC TAGS: Light scattering, fluorescence, Roman scattering, quantum theory, intermediate optical phenomena

ABSTRACT: The authors point out that the secondary emission can be described either in terms of quantum or classical theory, and in many cases it is advantageous to use a combination of elements of both theories. The applicability of the conceptions depends upon the relationship between the electron oscillator damping \mathcal{T} , the frequency of molecular vibrations ω , and the vibration damping Γ . Outside the resonance, the Roman scattering is well described by the classical model in which the molecular polarizability is a linear function of the nuclear coordinates. It is still applicable under resonance conditions if $\mathcal{T} \succ \omega \succ \Gamma$. When $\omega \succ \mathcal{T} \succ \Gamma$, the distinction between the free and the forced oscillations becomes

ACCESSION NR: AP4013327

questionable. Under these conditions, the polarizability conception is no more useful. Instead, a more general "transitional function" can be introduced which is used in radio electronics and in theory of oscillations. This function describes the general features of the spectra. Orig. art. has: 2 figures.

ASSOCIATION: Institut organicheskoy khimii Akademii Nauk SSSR (Institute for Organic Chemistry, Academy of Sciences SSSR)

SUBMITTED: 10Jul63

DATE ACQ: 26Feb64

ENCL: 00

SUB CODE: PH

NO REF SOV: 1006

OTHER: 000

Card 2/2

SHORYGIN, P.F.; ROSHCHOPKIN, V.P.; KHOMENKO, A.Kh.

Regularities in the mutual influence of atomic groups adjoinging the methylene bridge. Dokl. AN SSSR 159 no.2:391-394 N '64.

(MIRA 17:12)

1. Institut organicheskoy khimii im. N.D. Zelinskogo AN SSSR. Predstavleno akademikom A.N. Nesmeyanovym.

POPON, Yeams; EMOMERIKO, A.Kh.; SHORYCIN, F.F.

Optitizing of the vibration frequencies of multiple bonds of symmetrical molecules. inv. AN SSSR Ser. knim. no.1:51-52 165.

(MTRA 18:2)

1. Institut organicheskoy khimii im. N.D. Zelinskogo AN SSSR.

L 34880-65 EWT(1)/EWT(m)/EPF(c)/EWP(j)/EEC(t) Pc-4/Pr-4/Peb IJP(c) RM
ACCESSION NR: AP5005034 S/0051/65/018/002/0206/0211

AUTHOR: Ivanova, T. M.; Yanovskaya, L. A.; Shorygin, P. P.

TITLE: Spectra of resonant Reman scattering of polyene compounds having structural absorption bands

SOURCE: Optika i spektroskopiya, v. 18, no. 2, 1965, 206-211

TOPIC TAGS: Reman scattering, Reman spectrum, polyene compounds, diethyl ether, absorption band

ABSTRACT: This is a continuation of earlier work by two of the authors (Shorygin and Ivanova) on resonant Raman spectra of substances with large lifetimes of effective electron-vibrational levels. In the present article the authors report an investigation of Raman spectra of the vinylogous series of diethyl ethers of polyene a,ω-dicarboxylic acids C2H500C(CH=CH)nC00C2H5, n = 1--8, whose absorption bands have a pronounced vibrational structure. As n increases and the exciting frequency approaches the absorption band, the lines that become particularly strong in intensity in the Raman spectra are those with frequencies ~ 1140 and ~ 1550 cm-1

Card 1/2

L 34880-65
ACCESSION NR: AP5005034

Near resonance, progressions of the ~ 1140 and ~1550 cm⁻¹ vibrations and their different combinations appear in the scattering spectra, and under certain conditions of excitation, the intensity of the overtones exceeds the intensity of the fundamentals; in this respect, the scattering spectrum becomes similar to that of resonance fluorescence. It is shown that the frequency dependence of the line in-

tensities of the resonant Reman spectrum in the region of the structural absorption band is characterized by several maxima. Orig. art. has 1 figure and 4 tables.

ASSOCIATION: None

SUBMITTED: 28Nov63 ENCL: 00 ' SUB CODE: OP, OC

NR REF SOV: 006 OTHER: 004

Card 2/2

"APPROVED FOR RELEASE: 08/09/2001

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L 5424-66 EWT(1)/T IJP(c)

ACCESSION NR: AP5019766
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UR/0051/65/019/002/0289/0291

AUTHOR: Morozov, V. A.; Shorygin, P. P.

535.338.001.1

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TITIE: Contribution to the theory of radiative width of spectral lines

SOURCE: Optika i spektroskopiya, v. 19, no. 2, 1965, 289-291

21,44,55

TOPIC TAGS: spectral line, line width, photon, spectral energy distribution,

light emission

ABSTRACT: This is a continuation of earlier work [Abstracter's note: the reference to the earlier paper has been emitted from the source as a result of a printer's error], where a system of equations for the U matrix was derived with account of exchange of virtual photons between overlapping intermediate levels. The present paper considers the influence of this phenomenon on the change in the spontaneous-emission line shape. The spontaneous-emission line contours are calculated for a molecule with two close excited levels remote from the ground level, first neglecting and then taking into account an exchange of photons between the excited levels. Allowance for the exchange is shown to produce a noticeable shift in the line peak and a strong distortion of its symmetry. Orig. art. has: 3 figures and 15 formulas.

Card 1/2

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L 2127-66 EVT(1) ACCESSION NR: AP5025301

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sp. Y

AUTHOR: Krushinskiy, L. L.; Shorygin, P. P.

TITLE: The theory of line intensities in Raman spectra

SOURCE: Optika i spektroskopiya, v. 19, no. 4, 1965, 562-574

TOPIC TAGS: Raman scattering, line intensity, harmonic oscillator

ABSTRACT: This paper is the sixth in a series dealing with the Raman scattering theory published by the authors since 1961. A comparison is made between the quantum and classical theories of the line intensities of Raman scattering in different excitation regions. It is shown that away from the resonance the results of the two theories practically coincide. Near the absorption band the quantum treatment leads to a slightly different frequency dependence of the line intensity than does the classical approximation. In the resonance region a satisfactory coincidence of the results occurs only for large attenuation constants (exceeding the half-width of the vibrational structure of the absorption) of the electronic oscillator. For smaller constants, the classical model of the linear oscillator with periodically varying parameters leads to a rough qualitative agreement with the results of quantum mechanical calculations. Some of the conclusions obtained Card 1/2

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L41695-65. ENT(m)/EPF(c)/EPR/ENP(j)/EWA(c) Pc_4/Pr_4/Ps_4 RPL WW/RM ACCESSION NR: AP5008909 AUTHOR: Shorygin, P. P.; Roshchupkin, V. P.; Stolyarova, L. G. TITLE: Effect of substituents on systems of Pi bonds via a methylene bridge SOURCE: Zhurnal fizicheskoy khimii, v. 39, no. 3, 1965, 605-612 TOPIC TAGS: methylene bridge, Pi bond, ultraviolet absorption spectrum nitrile? ABSTRACT: The spectroscopic parameters of molecules of the type X-CH2GS N; X-CH2-CH2-C=N and X-B -C=N were compared in order to establish the similarian molecules with the groups X and CN. In addition, molecules with the sam differences in the influence of substituents (X) transmitted through different types of bridges between the groups X and CN. In addition, molecules with ferent types of bridges between the groups X and CN. In the X-CH2-CO-R (seeneral from the types of bridges were compared: X-CH2-C=N, X-CH2-CH2-CH2-CN-CH2-CH2-CH2-CN-CH2-CH2-CN-CN-CH2-CH2-CN-CN-CH2-CN-CN-CN-CN-CN-CN-CN-CN-CN-CN-CN-CN-CN-
X-CH ₂ -CH ₂ -C N and X In the influence X and CH ₂ -CH CH ₂ X-CH ₂ -CH In the X-CH ₂ -CH ties and differences in the influence X-CH ₂ -C X-CH ₂ -CH CH ₂ X-CH ₂ -Ph. In the X-CH ₂ -Ferent types of bridges between the groups of the type X-CH ₂ -Ph. In the X-CH ₂ -Ferent types of bridges were compared: X-CH ₂ -C X-CH ₂ -CH X-CH ₂ -Ph. In the X-CH ₂ -Ferent types of bridges X-CH ₂ -C X-CH ₂ -CH X-CH ₂ -Ph. In the X-CH ₂ -Ferent types of bridges X-CH ₂ -CH X-CH ₂ -CH X-CH ₂ -Ph. In the X-CH ₂ -Ferent types of bridges X-CH ₂ -CH X-CH ₂ -CH X-CH ₂ -CH X-CH ₂ -Ph. In the X-CH ₂ -Ferent types of bridges X-CH ₂ -CH X-CH ₂ -CH X-CH ₂ -CH X-CH ₂ -Ph. In the X

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ACC NR: AP600	06995 SO	URCE CODE: UR/OO5	51/66/020/002/021	4/0223	
AUTHORS: More	ozov, V. A.; S	horygin, P. P.		38	
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TITLE: Contribution of the	bution to the cules with cons	theory of resonar ideration of two	nt transformation intermediate end	n of ergy	
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TOPIC TAGS: action, light theory	light scatterin absorption, qu	ng, secondary emis nantum electrodyna	ssion, molecular amics, quantum f	inter- ield	
ABSTRACT: The into account the basis of the energy re	four of its ene the Heitler-Ma presentation fo	on of light by motor solution of the solution of the solution of the solution a system consister acting with it in this problem	Schrodinger equasting of a molecular (Proc. Roy. Ir	tion in ule and a	3
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ing in connection with the study of secondary emission modulation effects. Expressions are obtained for the intensity and shape of the absorbed and secondary radiation lines with allowance for virtual photon exchange between overlapping intermediate levels. In cases where this exchange is negligible, the resulting formulas coincide with similar ones of V. Weisskopf (Ann. Physik. v. 9, 23, 1931). The technique employed is compared with other quantum electrodynamic methods of considering this transformation of light by molecules. The relationship between absorbed and secondary radiation is discussed. The authors thank L. L. Krushinskiy and L. N. Ovander for a discussion of the results. Orig. art. has: 5 figures and 41 formulas.

SUB CODE: 20/ SUBM DATE: 30Nov64/ ORIG REF: 007/ OTH REF: 010

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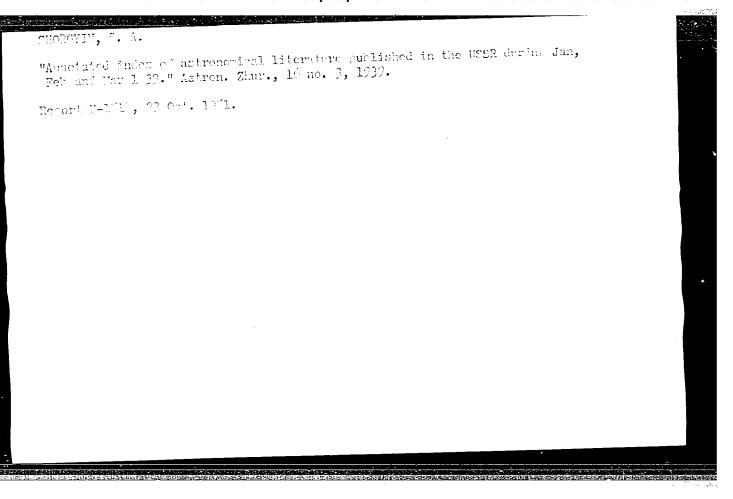
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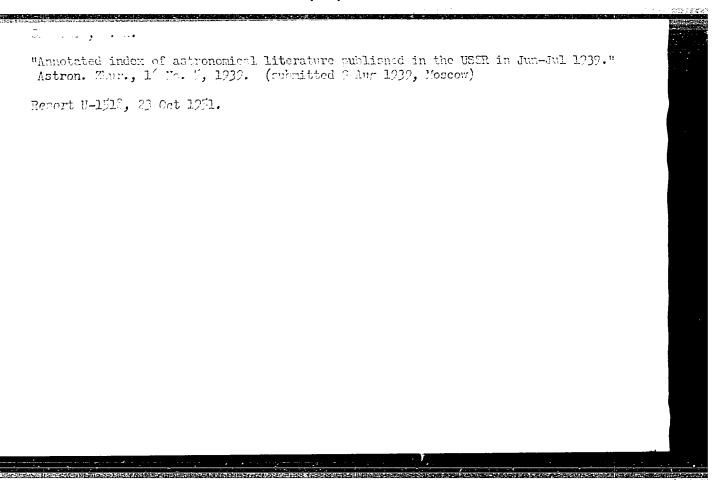
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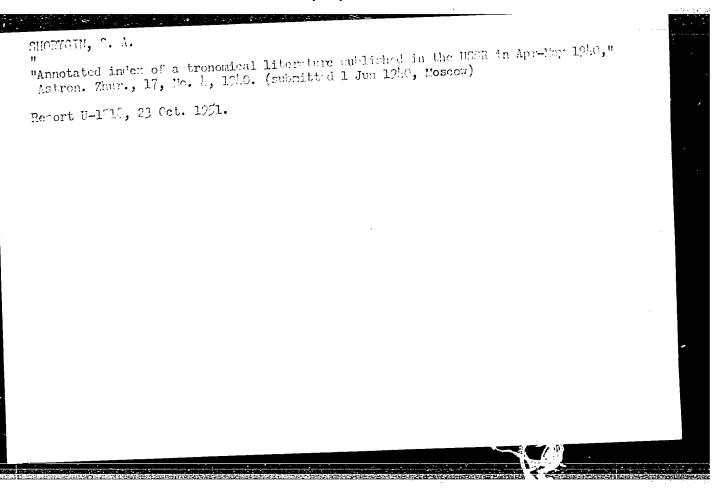
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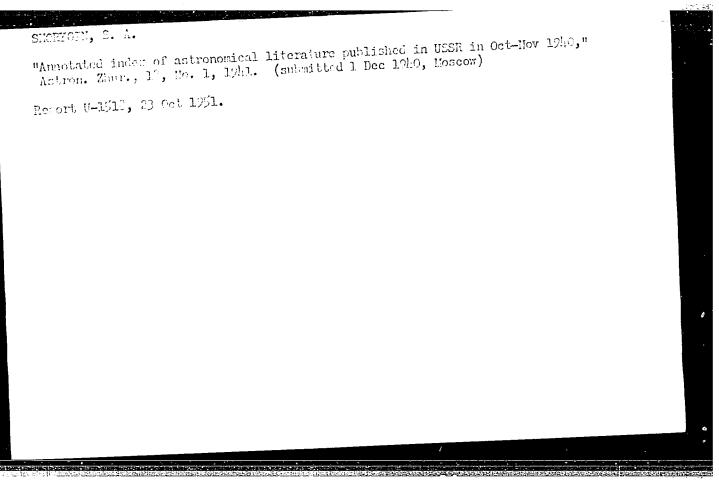
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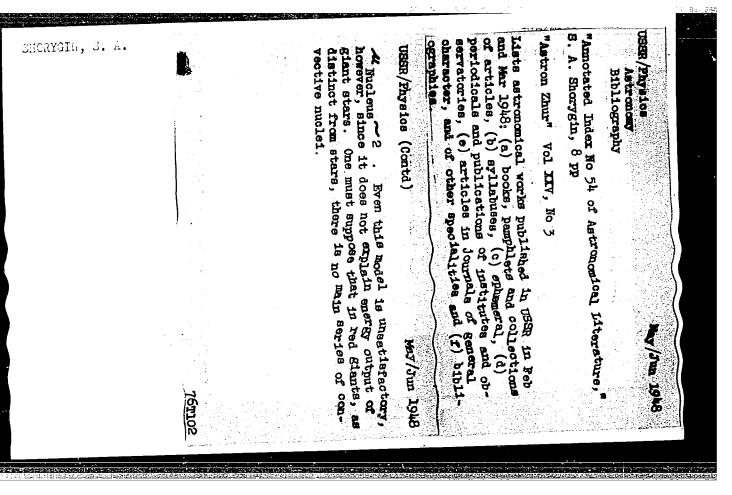
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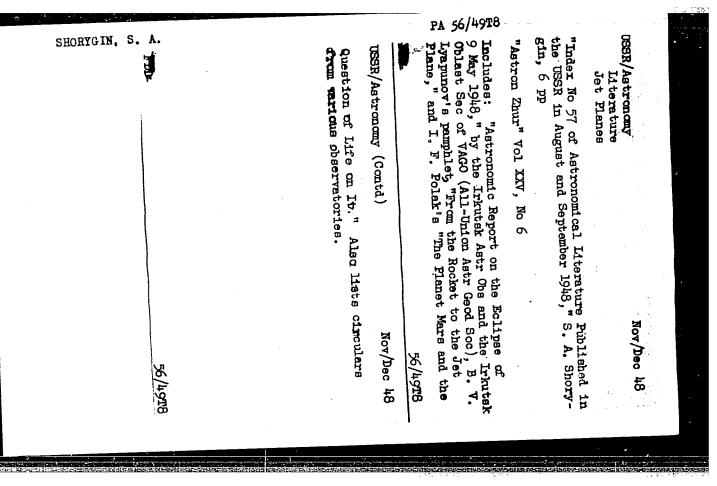
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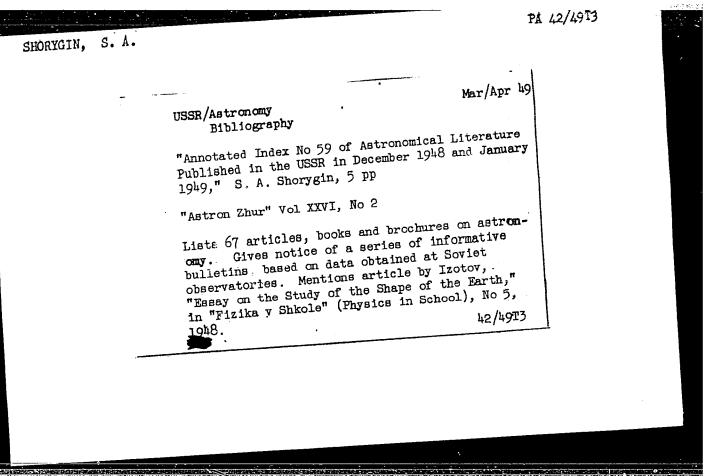
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