1969 SOUTHEASTERN SECTIONAL CONFERENCE

of

Undergraduate Student Chemists

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Hosted by the University of Alabama Chapter of the Student Affiliates of the American Chemical Society THE COLLISIONAL ENERGY TRANSFER PROBLEM AS STUDIED USING IODINE AND BROMINE.
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A literature search was conducted to determine the current state of knowledge concerning molecular collisions. For purposes of presentation, the search was narrowed to collisional energy transfer information contributed by work with iodine and bromine. Among the methods of characterizing the transfer of energy between molecules is to study the ability of chemically inert species to influence the rate of unimolecular reactions the ability of concerns the influence of inert gases on the recombination of iodine and bromine molecules. A brief discussion of the theoretical treatment given such studies by various investigators is included.

SEMI-EMPIRICAL MOLECULAR ORBITAL CALCULATIONS OF Cu(II) Chlorides Wroten McQuirter. Albert W. Schlueter, Tougaloo College, Tougaloo, Miss. and R. A. Jacobson, Dept. of Chem., Iowa State University, Ames, Iowa, toolo.

Sami-empirical molecular orbital calculations were carried out on ${\rm CuCl}_{4}$, ${\rm CuCl}_{5}$ —, and ${\rm Cu}_{2}{\rm Cl}_{6}$ — complexes. Good agreement with the observed spectra was found. A program was written to calculate the eigenvalues and eigenvector coefficients from which the allowed transitions were determined. The experimental parameters (F factors) were adjusted were determined. The experimental parameters (F factors) were adjusted for the observed spectrum of ${\rm CuCl}_{4}$ —, a square planar complex. The to fit the observed values, in paraenthesis observed values, were found following calculated vales, in paraenthesis observed values, were found for ${\rm F}_{6}$ =1.77, ${\rm F}_{-2}$ =2.00: 52,520 (51,000), 38,360 (41,500), 28,100 (29,500) for ${\rm F}_{6}$ =1.77, ${\rm F}_{-2}$ =2.00: 52,520 (51,000), 38,360 (41,500), 28,100 (29,500) for ${\rm F}_{6}$ =1.77, ${\rm F}_{-2}$ =2.00: 52,500). Other copper complexes were considered while the 25.38,(25,100(24,500)). Other copper complexes were considered while the 25.38,(25,100(24,500)). Other copper complexes were considered while the 25.38,(25,100(24,500)) at the above values. It was found that the calculated spectra were in excellent agreement with the observed spectra. It was further found if the 4d orbitals were included in the basis set that the d-d transitions were in fairly good agreement.

SYNTHESIS OF, Fe⁵⁵-LABELLED FERROCENE FOR USE IN ORBITAL ELECTRON CAPTURE RATIO MEASUREMENTS, Ronald P. Colle and R. W. Fink, School of Chemistry, Georgia Institute

of Technology, Atlanta, Georgia, 30332.

Tron-55 labelled ferrocene (bis-cyclopentadienyliron(II)) was synthesized for Iron-55 labelled ferrocene (bis-cyclopentadienyliron(II)) was synthesized for Several previous methods were evaluated with respect to the subsequent use of the Several previous methods were evaluated with respect to the subsequent use of the Sample as a vaporous source in a multiwire proportional counter [cf. Scobie, Moler, and Fink, Phys. Rev. 116, 657 (1959)]. The method chosen consisted of using anhydrous labelled FeCl₂ as the limiting reagent and reacting it with sodium cyclopentadienide in letrahydrofuran. After removal of the solvent by evaporation under reduced pressure, the ferrocene was removed from the reaction mixture and collected by sublimation. The labelled ferrous chloride was obtained by adding Fe55 activity (as FeCl, in HCl) to electrolytic iron powder and reacting the mixture with HCl. After removal of the water, electrolytic iron powder and reacting the mixture with HCl. After removal of the water, the salt was dehydrated to anhydrous FeCl₂ by heating in vacuo. This method permitted preparation of ferrocene with specific activities in the range of 2.5 µC/mg. The preparation of ferrocene with specific activities in the range of 2.5 µC/mg. The without having to separate and transfer reactants. The sample was contained in a without having to separate and transfer reactants. The sample was contained in a completely inert atmosphere from initial synthesis to final filling of the counter. Prior work on M/L orbital electron capture ratios has been summarized by Renier, et al. [Phys. Rev. 166, 935 (1968)] and by Fink [Phys. Rev. in press (1969)].

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SYNTHESIS OF Fe⁵⁵- LABELLED FERROCENE

FOR USE IN

ORBITAL ELECTRON CAPTURE RATIO MEASUREMENTS

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ABSTRACT

Iron-55 labelled ferrocene (bis-cyclopentadienyliron(II)) was synthesized for measurements of the M/L orbital electron capture ratio in the radioactive decay of Fe⁵⁵. Several previous methods were evaluated with respect to the subsequent use of the sample as a vaporous source in a multiwire proportional counter(cf. Scobie, Moler, and Fink, Phys. Rev. 116, 657 (1959)). The method chosen consisted of using anhydrous labelled FeClo as the limiting reagent and reacting it with sodium cyclopentadienide in tetrahydrofuran. After removal of the solvent by evaporation under reduced pressure, the ferrocene was removed from the reaction mixture and collected by sublimation. The labelled ferrous chloride was obtained by adding Fe⁵⁵ activity (as FeCl₃ in HCl) to electrolytic iron powder and reacting the mixture with HCl. After removal of the water, the salt was dehydrated to anhydrous FeCl2 by heating in vacuo. This method permitted preparation of ferrocene with specific activites in the range of 2.5 \(\mathcal{UC} \)/mg. The entire synthesis was conducted in a water- and air-free atmosphere and was effected without having to seperate and transfer reactants. The sample was contained in a completely inert atmosphere from initial synthesis to final filling of the counter. Prior work on M/L orbital electron capture ratios has been summarized by Renier, et. al. (Phys. Rev. 166, 935(1968)) and by Fink (Phys. Rev. in press (1969)).

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