

INTEROFFICE COMMUNICATION

Ponca City, Oklahoma
February 12, 1971

TO: Mr. R. H. Gerlach, Westlake, Louisiana

SUBJECT: PRELIMINARY DATA ON THE MASS SPEC-DISCLOSED R304 CATALYST SPECIES

To confirm our telecon of February 8 on the R304 catalyst species, I am attaching herewith some of Mr. Mynard Hamming's preliminary mass spec data which are to be completed and presented later in a formal research report, as per his report No. 839-0-3-71 on oxychlorination catalyst species. These data are taken from the R304 catalyst samples obtained by Dr. Martin C. Hawley and myself, and will be a part of our turnaround analysis report as per the last two turnaround studies. We have never analyzed for these R304 catalyst species before, as this is the first time (November 6, 1970 turnaround) that we have had access to a sampling of R304.

You may wish to consider the several process implications of these data prior to seeing Mynard's final report and our new turnaround study report. We have not tried to analyze these data, but plan to do so when all the present on-going R304 studies are complete. Also, by this preliminary data copy, we will ask Petrochemical Research for their mechanism interpretations of these anhydride structure formations and chemistry.



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Attachments

CC: CVF(2), FK(2), MCH, KRG,
HDB, LNV, JDM, HTF, MCHam,
GP, EAS

CCR 000008189

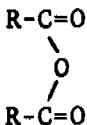
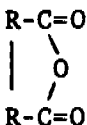
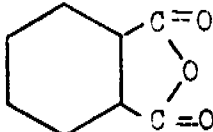
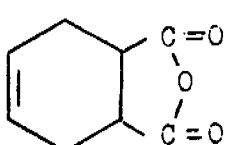
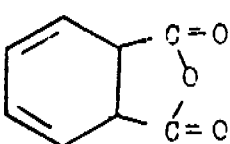
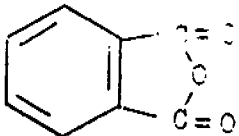
From Table 1 it can be noted that in going from succinic anhydride to phthalic anhydride (increasing number of double bonds in the hydrocarbon moiety) the concentration of anhydrides increases toward the bottom of the towel. (Not all samples have been examined.) It is also of interest to note that with the increase in concentration of anhydrides there is evidence of the anhydrides being converted to acids. The spectral evidence for acids is the appearance of the characteristic rearrangement peak of acids at m/e 88. The reaction of anhydrides with various hydrocarbons to form acids is a characteristic reaction of anhydrides (acidolysis of anhydrides). Additional proof of these components is being obtained by accurate mass measurements of several of the peaks on the mass spectra.

Several chloroparaffin components have been detected. These are shown in Table 2. The concentration of the chloroparaffins decreased in going toward the bottom of the reactor.

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TABLE 1

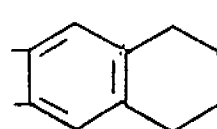
TYPES OF ANHYDRIDES DETECTED

General Formula and Structure	Molecular Ion Peak	Appearance
Type $C_n H_{2n-2} O_3$ 	<u>m/e</u> 130	Sample 54 (top of reactor) (low concentration)
Type $C_n H_{2n-4} O_3$  Succinic anhydride	<u>m/e</u> 128	Sample 54 (low concentration)
Type $C_n H_{2n-6} O_3$ 	<u>m/e</u> 154	Sample 55 (low concentration)
Type $C_n H_{2n-8} O_3$ 	<u>m/e</u> 152	Samples 56 and 57 (increasing concentration)
Type $C_n H_{2n-10} O_3$ 	<u>m/e</u> 150	Sample 58 (increasing concentration)
Type $C_n H_{2n-12} O_3$  Phthalic anhydride	<u>m/e</u> 148	Sample 59 (increasing concentration)

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TABLE 2

CHLOROPARAFFINS DETECTED IN SAMPLES

<u>Structure</u>	<u>Molecular Ion</u>
$ \begin{array}{c} \text{Cl} \quad \text{Cl} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{Cl} \quad \text{Cl} \end{array} $ Tetrachloroethylene	164
$ \begin{array}{c} \text{H} \quad \text{Cl} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{Cl} \quad \text{Cl} \end{array} $ Trichloroethylene	130
$ \begin{array}{c} \text{H} \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{Cl} \quad \text{Cl} \end{array} $ Dichloroethylene	96
$ \begin{array}{c} \text{H} \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{Cl} \end{array} $ (?)	$ \begin{array}{c} \text{H} \\ \\ \text{H} - \text{C} - \text{Cl} \\ \\ \text{H} \end{array} $ (?)
	$ \begin{array}{c} \text{Cl} \\ \\ \text{Cl} \end{array} $  (?)

These components are being checked by making accurate mass measurements.