A Brief Note on the Target Theory
By H. Eisenlohr
International Atomic Energy Agency, Vienna
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It is well known that the assumption of one-hit events on targets with equal volumes leads to a pure exponential dose effect relationship. There is, however, experimental evidence that more complicated situations may also show exponential dose effect relationships and, in fact, several results have been obtained to prove that an exponential dose effect relationship can be achieved by a suitable superposition of multiple hit functions.

In this note we will demonstrate, using a simple example, that an exponential dose effect relationship may also be obtained by a suitably chosen relation between the number of hits and the test effect within a target, which is subdivided into equal subvolumes.

Assume for simplicity a target consisting of two subvolumes $V_1$ and $V_2$ (later on we shall put $V_1 = V_2$). Let us consider three possibilities in establishing a dose effect relationship:

a) The test effect occurs if $V_1$ or $V_2$ or both have been hit; in this case the dose effect relationship is

$$W_a = 1 - e^{-VD},$$

where $D$ is the absorbed dose and $V = V_1 + V_2$.

b) The test effect occurs if both $V_1$ and $V_2$ have been hit:

$$W_b = 1 - e^{-V_1 D} - e^{-V_2 D} + e^{-VD};$$

c) The test effect occurs, definitely, if $V_1$ and $V_2$ have been hit. II. with a probability $p$, if $V_1$ or $V_2$ has been hit:

$$W_c = W_b + p (W_a - W_b)$$

$$= 1 + (p - 1) (e^{-V_1 D} + e^{-V_2 D}) + (1 - 2p) e^{-VD}.$$

If we put $p = 1/2$, $V_1 = V_2 = V$ in the last equation, we obtain

$$W_c = 1 - e^{-VD}.$$

Now

$$Z_1 = e^{-V_1 D}, \ Z_2 = e^{-V_1 D} + e^{-V_2 D} - 2 e^{-VD},$$

$$Z_2 = 1 - e^{-V_1 D} - e^{-V_2 D} + e^{-VD}$$

are the numbers of targets having obtained 0, 1, or 2 (one in $V_1$, one in $V_2$) hits respectively. Therefore, the last expression for $W_c$ is identical with $Z/2$, where

$$Z = Z_1 + 2 Z_2$$

is the mean number of hits per target. Hence, we may understand that, in case (c) also, a pure exponential dose effects relationship is obtained.

There is no difficulty to generalize this situation to cases with more than two subvolumes.


Reaktionen mit Acyl-isocyanaten
Von R. Neidlein
Pharmazeutisch-chemisches Institut der Universität Marburg/Lahn

Im Rahmen der Untersuchungen über Acyl-isocyanate war deren Reaktionsverhalten gegenüber Isotonitriilen in Gegenwart von Carbonsäuren von Interesse.

0,015 Mol eines entsprechenden Isotonitriils (I) und 0,016 Mol einer Carbonsäure (II), beispielsweise Benzoessäure, werden unter Kühlung (−2 bis −5 °C) in einem Gemisch von Äther/-Benzol (1 : 1) gelöst; wird dieses Reaktionsgemisch anschließend mit 0,015 Mol einer benzinolischen Lösung des Acyl-isocyanats (III) versetzt, so bilden sich in guten Ausbeuten durch innermolekulare Umacylierung gemischte Amide folgender Struktur:

$\begin{align*}
R - N - C - C - C - R' \\
\text{(I)} & \quad \text{H} & \quad \text{O} & \quad \text{H} & \quad \text{O} & \quad \text{C} & \quad \text{O} & \quad \text{R'} \\
\text{(II)} & \quad \text{O} & \quad \text{O} & \quad \text{C} & \quad \text{O} & \quad \text{R'} \\
\text{(III)} & \quad \text{O} & \quad \text{O} & \quad \text{O} & \quad \text{O} & \quad \text{R'}
\end{align*}$

$\text{(IV)}$

IV a) $R, R', R'' = \text{C}_4\text{H}_5$ —

IV b) $R = \text{C}_6\text{H}_{11}$; $R', R'' = \text{C}_6\text{H}_5$ —

IV a) $\text{C}_2\text{H}_4\text{N}_2\text{O}_4$ (372,4) Ausb.: 5,3 g (= 89% d. Th.), Schmp.: 166—167° (Zers.).

Ber. C 70,95 H 4,33 N 7,52,

Gef. C 71,06 H 4,52 N 7,40.

IV b) $\text{C}_2\text{H}_4\text{N}_2\text{O}_4$ (378,4) Ausb.: 4,5 g (= 75% d. Th.), Schmp.: 148—149° (Zers.).

Ber. C 69,83 H 5,86 N 7,40,

Gef. C 70,27 H 5,92 N 7,22.

Die Struktur der Verbindungen wurde durch Synthese bewiesen, IV a beispielsweise aus Oxalsäurechloridanilid und Dibenzamid.


2 R. Neidlein, Angew. Chem. 76, 596 [1964].
Di-isonitriles (V), for example 1,3-di-isonitrilo-cyclohexane, can be synthesized in a similar manner to bifunctional amides of the general structure (VI) as follows:

\[
2 \text{R'}' - \text{COOH} + 2 \text{R''}'' - \text{C} - \text{N} = \text{C} = \text{O} + \text{R''}'' \quad \text{N} = \text{C} \quad (V)
\]

\[
\text{R''}'' - \text{C} - \text{N} - \text{C} - \text{C} - \text{N} - \text{R}'''' - \text{N} - \text{C} - \text{C} - \text{N} - \text{C} - \text{R}''
\]

(CVI)

The binuclear cyclopentadienylmetal carbonyls \([\text{C}_6\text{H}_5\text{Mo(CO)}_2]_2\), \([\text{C}_6\text{H}_5\text{M(CO)}_2]_2\) (M = Fe and Ru), and \([\text{C}_6\text{H}_5\text{MCOI}]_2\) (M = Ni and Pt) all react with iodine via cleavage of the metal-metal bond but without carbon monoxide evolution to form the mononuclear iodo complexes \(\text{C}_6\text{H}_5\text{M}(\text{CO})_4\text{I}\), \(\text{C}_6\text{H}_5\text{M}(\text{CO})_4\text{I}\) (M = Fe and Ru), and \(\text{C}_6\text{H}_5\text{MCOI}\) (M = Ni and Pt), respectively. I have now found that the mononuclear cyclopentadienylcobalt dicarbonyl, \(\text{C}_6\text{H}_5\text{Co(CO)}_2\), also reacts readily with iodine in diethyl ether solution at room temperature evolving carbon monoxide and precipitating black crystalline cyclopentadienylcobalt carbonyl diiodide, \(\text{C}_6\text{H}_5\text{CoCOI}_2\) (Anal.: Calcd.: C, 26.3; H, 1.2; Co, 4.4; I, 49.0; mol. wt., 406. Found: C, 18.3; H, 1.3; Co, 1.6; I, 49.0; mol. wt., 398 [osmometer in benzene solution]).

Cyclopentadienylcobalt carbonyl diiodide forms black crystals sparingly soluble in pentane and diethyl ether but more soluble in dichloromethane, benzene, and tetrahydrofuran to give deep purple solutions. It cannot be sublimed by heating at 0.1 mm. Its infrared spectrum exhibits a sharp strong band at 2068 cm\(^{-1}\) (Halocarbon oil null) due to the single carbonyl group. Its proton n.m.r spectrum exhibits a single resonance at \(\tau 4.35\) due to the five equivalent \(\pi\)-cyclopentadienyl protons.


The single carbonyl group in \(\text{C}_6\text{H}_5\text{CoCOI}_2\) is readily displaced by amines and phosphines in solution at room temperature. For example, \(\text{C}_6\text{H}_5\text{CoCOI}_2\) reacts with excess pyridine in benzene solution at room temperature with gas evolution and the precipitation of black \(\text{C}_6\text{H}_5\text{Co}(\text{C}_6\text{H}_5\text{N})_2\) (Anal.: Calcd.: C, 26.3; H, 2.2; Co, 12.9; N, 3.1; I, 55.6. Found: C, 27.0; H, 2.1; Co, 12.7; N, 3.0; I, 55.2). This black solid is less soluble than \(\text{C}_6\text{H}_5\text{CoCOI}_2\) in benzene but gives dark green non-conducting solutions in acetone. Under similar conditions triphenylphosphine forms dark green \(\text{C}_6\text{H}_5\text{CoP(C}_6\text{H}_5)_3\). However, aliphatic amines such as ethylenediamine and diethylenetriamine react with \(\text{C}_6\text{H}_5\text{CoCOI}_2\) to form tan solids sparingly soluble even in tetrahydrofuran. Unlike the other cobalt derivatives discussed in this note, these tan compounds are very sensitive to the moisture of the air and have not yet been obtained pure.

The reaction of \(\text{C}_6\text{H}_5\text{Co}(\text{CO})_4\) with iodine to give \(\text{C}_6\text{H}_5\text{CoCOI}_2\) is entirely analogous to the reaction of \(\text{Fe(CO)}_5\) with iodine to give \(\text{Fe(CO)}_4\text{I}\) thus demonstrating further the previously observed analogy between the chemistry of cyclopentadienylcobalt carbonyl and iron pentacarbonyl. The compound \(\text{C}_6\text{H}_5\text{CoCOI}_2\) is also closely related to the perfluoroalkyl derivatives \(\text{C}_6\text{H}_5\text{CoCOR}^1\).

Further studies on \(\text{C}_6\text{H}_5\text{CoCOI}_2\) are in progress and will be reported in detail in the future.

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