Note on the Structures of the Gallium and Indium Trihalides

BY D. P. STEVENSON[1] AND VERNER SCHOMAKER

Brode[2] recently published the results of an electron-diffraction investigation of the structures of the so-called trihalides of aluminum, gallium and indium. We believe that the interatomic distances which he reported (given in row *a* of the table) have been falsified by his application of an unsuitable "correction,"[3] and that the values given below in rows *b* and *c* are significantly more reliable. Row *b* gives the values found by Brode with the use of the usual correlation method[4] (omitting the Wierl correction), while those of row *c* are the ones we have obtained by the application of the radial distribution method[5] to his data. These two sets of values agree reasonably well except in the case of Ga_2Br_6.

TABLE I

AVERAGE M–X BOND LENGTHS IN THE TRIHALIDES OF GALLIUM AND INDIUM

		Cl	Br	I
Ga	[a]	2.16	2.35	2.40[d]
	[b]	2.22	2.41	2.48
	[c]	2.22	2.34	2.50
In	[a]	2.39	2.49	2.67
	[b]	2.46	2.56	2.76
	[c]	2.46	2.58	2.76

[a] Brode's "corrected" value. [b] Brode's uncorrected value. [c] From the first peaks of the radial distribution functions. [d] GaI_3, coplanar equilateral triangle.

The bond angle values (∠ XMX) indicated by the relative positions of the first and second maxima of the radial distribution functions substantiate Brode's conclusion that under the conditions of his experiments gallium tri-iodide is monomeric and coplanar, whereas the five other trihalides are dimeric. Inasmuch as we could not take account of the minima, for which Brode reported no measurements, the radial distribution functions tend to show spurious features, in these cases beyond the first two peaks, and we can draw no conclusions with regard to the conformation of the dimers.

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(2) Brode, *Ann. Physik*, **37**, 344 (1940).

(3) The correction is one due to Wierl (*ibid.*, **8**, 521 (1931)), and implies a procedure of measurement different from that which has been found suitable by Pauling and his co-workers. Almost certainly this correction should not have been applied to Brode's measurements, for his measurements on aluminum chloride agree well with those reported by Palmer and Elliott (THIS JOURNAL, **60**, 1852 (1938)).

(4) L. Pauling and L. O. Brockway, *J. Chem. Phys.*, **2**, 867 (1934).

(5) L. Pauling and L. O. Brockway, THIS JOURNAL, **57**, 2684 (1935); V. Schomaker, A. C. S. meeting, Baltimore, Md., April, 1939.

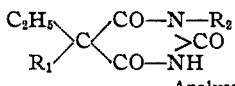
NEW COMPOUNDS

Some N-Aralkyl Barbituric Acids

The N-benzyl and N-phenethyl derivatives of amytal and neonal have been prepared by conventional methods from the corresponding malonic esters and benzyl and phenethyl ureas. They were crystallized from hexane. Data on these substances are presented in the table. The benzyl and phenethyl nembutals were also prepared, but, although general identity was shown by analysis, they were not obtained in a satisfactorily homogeneous condition.

TABLE I

1-ARALKYL-5-ETHYL-5-ALKYL BARBITURIC ACIDS



R_1	R_2	M. p., °C.	Formula	Analyses, % Calcd. C	Calcd. H	Found C	Found H
n-C_4H_9	$C_6H_5CH_2$	64	$C_{17}H_{22}O_3N_2$	67.50	7.34	67.79	7.59
n-C_4H_9	$C_6H_5CH_2CH_2$	74	$C_{18}H_{24}O_3N_2$	68.31	7.64	68.76	7.83
i-C_5H_{11}	$C_6H_5CH_2$	87–88	$C_{18}H_{24}O_3N_2$	68.31	7.64	68.38	7.56
i-C_5H_{11}	$C_6H_5CH_2CH_2$	106–107	$C_{19}H_{26}O_3N_2$	69.05	7.93	69.18	7.87

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Chaulmoogryl Quaternary Salts[1]

Since favorable bacteriological results have been obtained with methiodides and benzochlorides from mixtures of chaulmoogryl and hydnocarpyldimethylamines, it was decided to prepare some pure substances of this type.

Chaulmoogryl bromide[2] was heated in a bomb-tube at 105–110° with 33% methanolic dimethylamine in excess.

(1) Dittmar, *Z. Krebsforsch.*, **49**, 515 (1939), mentions a "Chaulmoogryl Zephirol." So far as the authors know these compounds have not been described.

(2) Sacks and Adams, THIS JOURNAL, **48**, 2397 (1926).