but its greatest value is in the ability to extend limited experimental data to much wider temperature ranges and in the prediction of values for structurally similar chemicals for which no experimental values exist. Detailed tabulations with eq 2 have been prepared by the author under the sponsorship of ESDU and may be found in ref 3-6 for 58 alkanes, 27 alkenes and dienes, 166 halogenated aliphatic hydrocarbons, and 146 *n*-alkyl esters. New experimental measurements have also been made with 6 aliphatic ethers and a more detailed description is given in ref 7 of the quality of fit of eq 2 to the experimental values.

4 Conclusions

An equation has been developed which fits the experimental thermal conductivity data from the melting point to approximately 0.9 of the critical temperature. The constants of this equation were correlated not only as individual compounds but also as members of their chemical series, and the values tabulated by this procedure represent the thermal conductivity data to within their estimated experimental accuracy. The predicted data obtained by interpolation of the constants of eq 2 are claimed to have a similar accuracy which is much better than would have been obtained from any purely predictive equation of the type described in ref 8.

Acknowledgment

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Received for review September 5, 1978. Accepted March 7, 1979.

NEW COMPOUNDS

Synthesis of *N*-(1-Naphthyl) Hydroxamic Acids

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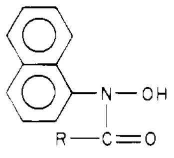
Preparation and properties of eight new crystalline *N*-aryl hydroxamic acids derived from *N*-(1-naphthyl)hydroxylamine are described.

Introduction

Synthesis of ten hydroxamic acids, of which eight are new acids, derived from *N*-(1-naphthyl)hydroxylamine with the general formula (I) (where R is acetic or substituted benzoic acid derivatives), is described.



I

Table I. Properties of *N*-(1-Naphthyl) Hydroxamic Acids[a]

compd no.	hydroxamic acid	mol formula	mp, °C	% yield	IR spectra, cm^{-1} ν_{O-H}	IR spectra, cm^{-1} $\nu_{C=O}$	IR spectra, cm^{-1} ν_{N-O}	UV spectra (λ_{max}), nm band II	UV spectra (λ_{max}), nm band I
I	*N*-(1-naphthyl)benzo-	$C_{17}H_{13}NO_2$	165	70	3222	1626	905	275	225
II	*N*-(1-naphthyl)aceto-	$C_{12}H_{11}NO_2$	120	65	3297	1626	905	284	224
III	*N*-(1-naphthyl)cinnamo-	$C_{19}H_{15}NO_2$	130	75	3190	1626	922	285	220
IV	*N*-(1-naphthyl)-*p*-chlorobenzo-	$C_{17}H_{12}NO_2Cl$	148[b]	60	3279	1653	910	282	236
V	*N*-(1-naphthyl)-*o*-chlorobenzo-	$C_{17}H_{12}NO_2Cl$	126	55	3270	1650	920	283	225
VI	*N*-(1-naphthyl)-*p*-bromobenzo-	$C_{17}H_{12}NO_2Br$	207	60	3190	1626	903	283	224
VII	*N*-(1-naphthyl)-*p*-iodobenzo-	$C_{17}H_{12}NO_2I$	175[c]	65	3248	1623	904	283	224
VIII	*N*-(1-naphthyl)-*p*-nitrobenzo-	$C_{17}H_{12}N_2O_4$	174	70	3215	1653	909	257	224
IX	*N*-(1-naphthyl)-*m*-nitrobenzo-	$C_{17}H_{12}N_2O_4$	138	65	3221	1653	909	283	226
X	*N*-(1-naphthyl)-3,5-dinitrobenzo-	$C_{17}H_{11}N_3O_6$	215	60	3248	1639	905	267	224

[a] Elemental analysis in agreement with theoretical values were obtained and submitted for review. [b] Reported mp 148 °C (*5*). [c] Reported mp 175 °C (*5*).

The physical properties of *N*-(1-naphthyl) hydroxamic acids are given in Table I. All the hydroxamic acids are reported for the first time except the *p*-nitro- and *p*-chloro-substituted acids which were reported earlier (*5*). All these acids are white crystalline compounds except the nitro- and iodo-substituted acids which are yellow and pink, respectively. They are sparingly soluble in water but readily soluble in benzene, ethyl alcohol, dioxane, diethyl ether, and chloroform.

The presence of an O–H stretching band is assigned in the region about 3200 cm^{-1} and in conformity with the reported value (*1*, *2*, *6*, *8*, *9*). The lower shift of the O–H band was due to the intramolecular hydrogen bonding of the $-OH\cdots C{=}O$. The C=O and N—O bands are assigned at about 1630 and 920 cm^{-1}, respectively.

In the ultraviolet region two characteristic naphthalene bands, I and II, are observed at 225 and 270 nm, respectively. The assignment of these bands is supported by comparing the related compounds (*7*, *10*). In the *N*-(1-naphthyl) hydroxamic acids, the ratio of bands II and I, λ_{II}/λ_{I}, is generally found at about 1.22 (*3*, *4*).

A typical preparation of *N*-(1-naphthyl)benzohydroxamic acid is given below.

The *N*-(1-naphthyl)hydroxylamine was prepared as described elsewhere (*5*). Into a 500-mL three-necked flask equipped with stirrer, dropping funnel, and thermometer, 100 mL of diethyl ether, 10.9 g (0.1 mol) of freshly crystallized (1-naphthyl)-hydroxylamine, and a fine suspension of 12.6 g (0.15 mol) of sodium bicarbonate in 25 mL of water were added. After the mixture was cooled to 0 °C or lower, 9.5 g (0.1 mol) of benzoyl chloride dissolved in 100 mL of diethyl ether was added dropwise over a period of 20–30 min. Some of the product was precipitated as light yellowish solid while the ether layer was separated and ether removed under vaccum. The light yellow residue was combined with the precipitated solid, triturated for about 15 min on a glass mortar with a saturated solution of a sodium bicarbonate to remove the acid impurities, filtered, and washed with cold water. The yield of air-dried product, mp 160 °C, was 70%. Two crystallizations from a mixture of benzene and petroleum ether without the use of charcoal gave white needles, mp 165 °C.

Acknowledgment

We are indebted to Professor A. S. Kapur and Dr. S. D. Nigam, Government Science College, Satna, and are thankful to the authorities of the National Chemical Laboratories of Poona for spectral measurements and microanalysis of samples.

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Received for review August 25, 1978. Accepted March 6, 1979. Grateful acknowledgment is made to the U.G.C., New Delhi, for financial assistance.

Synthesis of Novel Energetic Aliphatic Compounds

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Reported here are the syntheses and physical properties of nine novel azides containing other energetic groups. These groups include nitramines, nitro nitramines, nitro esters, nitro ethers, nitrate esters, and (difluoroamino)alkanes. In addition, two new energetic fluorodinitro formals are reported.

The chemistry of aliphatic azido compounds is extensive, dating back to the work of Curtius in 1901. The principal chemical effort, particularly in recent years, has been directed at improving the methods of synthesis rather than the synthesis of new azides. These methods of improvement have included a better choice of leaving groups, reaction solvents, and/or catalysts. A comprehensive account of the chemistry of the azido group has recently been published (*1*). We are extending the synthetic chemistry of aliphatic azides to include other energetic groups. These groups include nitramines, nitro nitramines, nitro esters, nitro ethers, nitrate esters, and (difluoroamino)alkanes. The following nine new azides show the incorporation of these groups.

An example of a nitramine azide is 1,3-diazido-2-nitrazapropane (I) which was prepared by the reaction of sodium azide with 1,3-dichloro-2-nitrazapropane (*2*).

$$\mathrm{N(NO_2)[CH_2Cl]_2 + 2NaN_3 \rightarrow \underset{I}{N(NO_2)[CH_2N_3]_2}}$$

A nitro nitramine azide, *N*-(trinitroethyl)-*N*-(3-azidopropyl)nitramine (III), was prepared by the nitration of *N*-(trinitroethyl)-*N*-(3-azidopropyl)amine (II) with nitric acid–acetic acid. II was obtained by the reaction of (3-azidopropyl)amine hydrochloride with trinitroethanol.

$$\mathrm{(NO_2)_3CCH_2OH + N_3CH_2CH_2CH_2NH_2{\cdot}HCl \rightarrow \underset{II}{(NO_2)_3CCH_2NHCH_2CH_2CH_2N_3}}$$

$$\mathrm{II + HNO_3\text{–}Ac_2O \rightarrow \underset{III}{(NO_2)_3CCH_2N(NO_2)CH_2CH_2CH_2N_3}}$$

The nitro azido esters prepared were 1,3-diazido-2-propyl-4,4,4-trinitrobutyrate (IV), 1,3-diazido-2-propyl-4,4,4-fluorodinitrobutyrate (V), and bis(1,3-diazido-2-propyl)oxalate (VI). IV was obtained from the reaction of 4,4,4-trinitrobutyryl chloride with 1,3-diazido-2-propanol (*3*).

$$\mathrm{(NO_2)_3CCH_2CH_2COCl + HOCH(CH_2N_3)_2 \rightarrow \underset{IV}{(NO_2)_3CCH_2CH_2CO_2CH(CH_2N_3)_2}}$$

V was prepared from 4,4,4-fluorodinitrobutyryl chloride and 1,3-diazido-2-propanol.

$$\mathrm{F(NO_2)_2CCH_2CH_2COCl + HOCH(CH_2N_3)_2 \rightarrow \underset{V}{F(NO_2)_2CCH_2CH_2CO_2CH(CH_2N_3)_2}}$$

VI was synthesized from oxalyl chloride and 1,3-diazido-2-propanol.

$$\mathrm{[COCl]_2 + 2HOCH(CH_2N_3)_2 \rightarrow \underset{VI}{[CO_2CH(CH_2N_3)_2]_2}}$$

The nitro azido ethers prepared were 1,3-diazido-2-propyl-fluorodinitroethyl formal (VII) and 1,2-diazido-3-fluorodinitroethoxypropane (VIII). VII was obtained from the reaction of

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